

10/ 562,112

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LOGINID:sssptal202txn

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	NOV 21	CAS patent coverage to include exemplified prophetic substances identified in English-, French-, German-, and Japanese-language basic patents from 2004-present
NEWS	3	NOV 26	MARPAT enhanced with FSORT command
NEWS	4	NOV 26	CHEMSAFE now available on STN Easy
NEWS	5	NOV 26	Two new SET commands increase convenience of STN searching
NEWS	6	DEC 01	ChemPort single article sales feature unavailable
NEWS	7	DEC 12	GBFULL now offers single source for full-text coverage of complete UK patent families
NEWS	8	DEC 17	Fifty-one pharmaceutical ingredients added to PS
NEWS	9	JAN 06	The retention policy for unread STNmail messages will change in 2009 for STN-Columbus and STN-Tokyo
NEWS	10	JAN 07	WPIDS, WPINDEX, and WPIX enhanced Japanese Patent Classification Data
NEWS	11	FEB 02	Simultaneous left and right truncation (SLART) added for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS	12	FEB 02	GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS	13	FEB 06	Patent sequence location (PSL) data added to USGENE
NEWS	14	FEB 10	COMPENDEX reloaded and enhanced
NEWS	15	FEB 11	WTEXTILES reloaded and enhanced
NEWS	16	FEB 19	New patent-examiner citations in 300,000 CA/CAPLUS patent records provide insights into related prior art
NEWS	17	FEB 19	Increase the precision of your patent queries -- use terms from the IPC Thesaurus, Version 2009.01
NEWS	18	FEB 23	Several formats for image display and print options discontinued in USPATFULL and USPAT2
NEWS	19	FEB 23	MEDLINE now offers more precise author group fields and 2009 MeSH terms
NEWS	20	FEB 23	TOXCENTER updates mirror those of MEDLINE - more precise author group fields and 2009 MeSH terms
NEWS	21	FEB 23	Three million new patent records blast AEROSPACE into STN patent clusters

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,  
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS LOGIN Welcome Banner and News Items

NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 11:39:56 ON 23 FEB 2009

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.22	0.22

FILE 'REGISTRY' ENTERED AT 11:40:15 ON 23 FEB 2009

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 FEB 2009 HIGHEST RN 1109311-46-7

DICTIONARY FILE UPDATES: 20 FEB 2009 HIGHEST RN 1109311-46-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10562112d.str





```

chain nodes :
7  8  9  10  11  14  28  29  30
ring nodes :
1  2  3  4  5  6  16  17  18  19  20  21  22  23  24  25
chain bonds :
2-7  3-14  6-11  7-8  8-9  8-10  17-29  19-28  24-30
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  16-17  16-21  17-18  18-19  19-20  20-21  20-22
21-25  22-23  23-24  24-25
exact/norm bonds :
2-7  3-14  6-11  7-8  8-9  8-10  16-17  16-21  17-18  17-29  18-19  19-20  19-28
24-30
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  20-21  20-22  21-25  22-23  23-24  24-25

```

G1: Ak, H

G2: H, CN, X

```

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS
11:CLASS 14:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom 25:Atom 28:CLASS 29:CLASS 30:CLASS
fragments assigned product role:
containing 16
fragments assigned reactant/reagent role:
containing 1

```

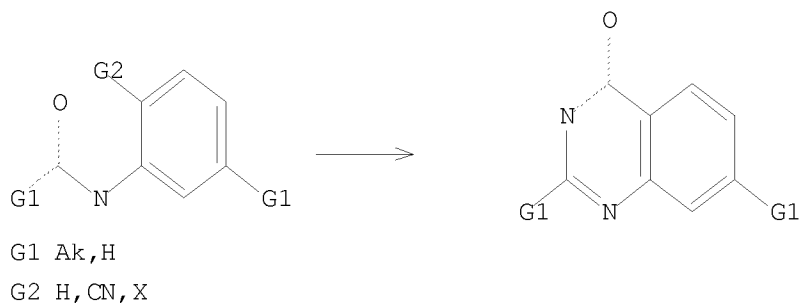
L1 STRUCTURE UPLOADED

=> d L1

L1 HAS NO ANSWERS

L1 STR

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Structure attributes must be viewed using STN Express query preparation.

=> file casreact  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.96	1.18

FULL ESTIMATED COST

FILE 'CASREACT' ENTERED AT 11:41:31 ON 23 FEB 2009  
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FILE CONTENT:1840 - 19 Feb 2009 VOL 150 ISS 2

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\*\*\*\*\*  
\* CASREACT now has more than 16.5 million reactions \*  
\* \*  
\*\*\*\*\*

CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 11:39:56 ON 23 FEB 2009)

FILE 'REGISTRY' ENTERED AT 11:40:15 ON 23 FEB 2009

L1 STRUCTURE UPLOADED

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FILE 'CASREACT' ENTERED AT 11:41:31 ON 23 FEB 2009

=> s l1

SAMPLE SEARCH INITIATED 11:41:42 FILE 'CASREACT'  
SCREENING COMPLETE - 2101 REACTIONS TO VERIFY FROM 141 DOCUMENTS  
  
100.0% DONE 2101 VERIFIED 106 HIT RXNS 12 DOCS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED VERIFICATIONS: 39274 TO 44766  
PROJECTED ANSWERS: 33 TO 447

L2 12 SEA SSS SAM L1 ( 106 REACTIONS)

=> s l1 full

FULL SEARCH INITIATED 11:41:51 FILE 'CASREACT'  
SCREENING COMPLETE - 40457 REACTIONS TO VERIFY FROM 2766 DOCUMENTS  
  
100.0% DONE 40457 VERIFIED 2129 HIT RXNS 258 DOCS  
SEARCH TIME: 00.00.04

L3 258 SEA SSS FUL L1 ( 2129 REACTIONS)

=> d l3 1- ibib abs hitrxn

'HITRXN' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS ----- GI and AB  
ALL ----- BIB, AB, IND, RE, Single-step Reactions  
APPS ----- AI, PRAI  
BIB ----- AN, plus Bibliographic Data  
CAN ----- List of CA abstract numbers without answer numbers  
CBIB ----- AN, plus Compressed Bibliographic Data  
DALL ----- ALL, delimited (end of each field identified)  
IABS ----- ABS, indented with text labels  
IALL ----- ALL, indented with text labels  
IBIB ----- BIB, indented with text labels  
IND ----- Indexing data  
IPC ----- International Patent Classifications  
ISTD ----- STD, indented with text labels  
OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels  
  
SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations  
  
MAX ----- Same as ALL  
PATS ----- PI, SO  
SCAN ----- TI and FCRD (random display, no answer number. SCAN  
must be entered on the same line as DISPLAY, e.g.,  
D SCAN.)  
SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for  
all single-step reactions)  
STD ----- BIB, IPC, and NCL  
  
CRD ----- Compact Display of All Hit Reactions  
CRDREF ----- Compact Reaction Display and SO, PY for Reference

FHIT ----- Reaction Map, Diagram, and Summary for first  
 hit reaction  
 FHITCBIB --- FHIT, AN plus CBIB  
 FCRD ----- First hit in Compact Reaction Display (CRD) format  
 FCRDREF ---- First hit in Compact Reaction Display (CRD) format with  
 CA reference information (SO, PY). (Default)  
 FPATH ----- PATH, plus Reaction Summary for the "long path"  
 FSPATH ----- SPATH, plus Reaction Summary for the "short path"  
 HIT ----- Reaction Map, Reaction Diagram, and Reaction  
 Summary for all hit reactions and fields containing  
 hit terms  
 OCC ----- All hit fields and the number of occurrences of the  
 hit terms in each field. Includes total number of  
 HIT, PATH, SPATH reactions. Labels reactions that have  
 incomplete verifications.  
 PATH ----- Reaction Map and Reaction Diagram for the "long  
 path". Displays all hit reactions, except those  
 whose steps are totally included within another hit  
 reaction which is displayed  
 RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)  
 RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)  
 RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)  
 RXS ----- Hit Reaction Summarizers (Map and Summary for all hit reactions)  
 SPATH ----- Reaction Map and Reaction Diagram for the "short  
 path". Displays all single step reactions which  
 contain a hit substance. Also displays those  
 multistep reactions that have a hit substance in both  
 the first and last steps of the reaction, except for  
 those hit reactions whose steps are totally included  
 within another hit reaction which is displayed

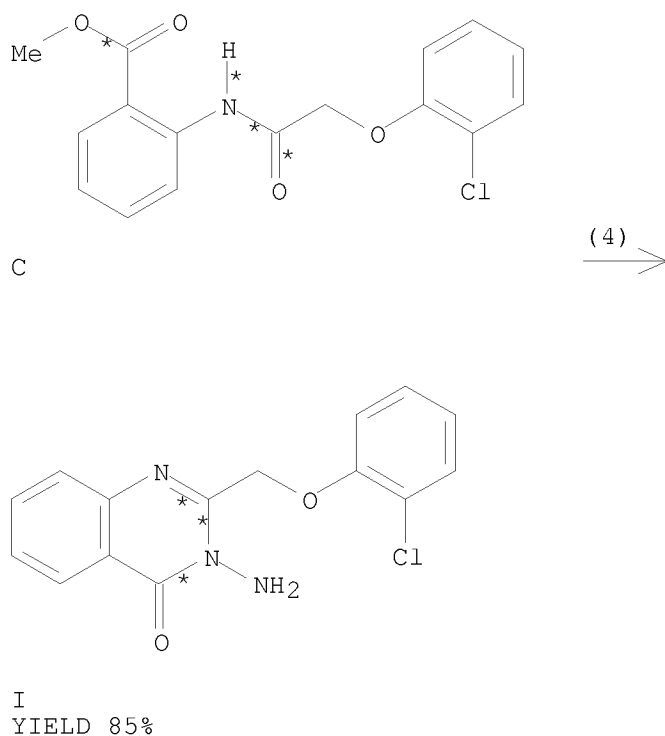
To display a particular field or fields, enter the display field  
 codes. For a list of the display field codes, enter HELP DFIELDS  
 at an arrow prompt (=>). Examples of combinations include: D TI;  
 D BIB RX; D TI, AU, FCRD. The information is displayed in the same order  
 as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH,  
 FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may  
 be used with the DISPLAY command to display the record for a specified  
 Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):ibib abs rx  
 YOU HAVE REQUESTED DATA FROM 258 ANSWERS - CONTINUE? Y/(N):y

L3 ANSWER 1 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 149:402296 CASREACT  
 TITLE: Synthesis and antimicrobial activity of some novel  
 2,3-disubstituted quinazolin-4(3H)ones  
 AUTHOR(S): Abbas, Safinaz E. S.; Saafan, Amal E. M.  
 CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of  
 Pharmacy, Cairo University, Egypt  
 SOURCE: Bulletin of Pharmaceutical Sciences, Assiut University  
 (2007), 30(1), 51-62  
 CODEN: BPAUEC; ISSN: 1110-0052  
 PUBLISHER: Assiut University Press  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB 3-Amino-2-(substituted phenoxyethyl/propyl)quinazolin-4(3H)ones (I) have  
 been prepared Refluxing I with 5-nitro-2-furaldehyde or 4-nitrobenzaldehyde  
 afforded the corresponding methyldienamines. Reaction of I with isatin

yielded the indolylideneamino derivs. Refluxing I with ofloxacin acid chloride furnished the corresponding carboxamides. Reaction of chloroacetyl chloride with I produced the 3-chloroacetyl amino derivative 9 which upon further reaction with the potassium salts of some antibacterial acids gave the corresponding carboxylate derivs. Sixteen compds. were screened for their antibacterial and antifungal activities. Thirteen compds. were found to possess high to moderate activity against *Pseudomonas aeruginosa* and some of them were also active against *Escherichia coli*. Only one compound was found to exhibit moderate antifungal activity against *Candida albicans*.

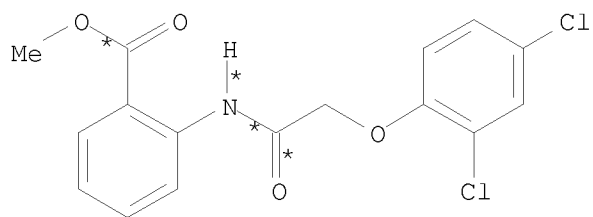
RX(4) OF 60      ...C ==> I...



RX(4)      RCT    C 301678-87-5  
              RGT    J 302-01-2 N2H4  
              PRO    I 1063716-09-5  
              SOL    71-36-3 BuOH  
              CON    8 - 10 hours, reflux

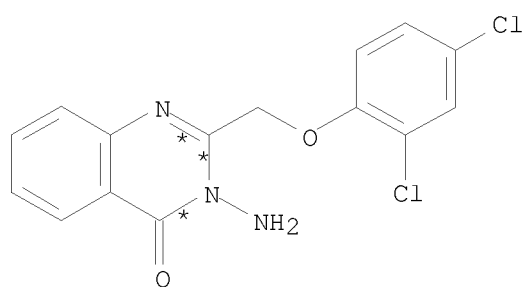
RX(5) OF 60      ...F ==> L...

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F

(5)  $\longrightarrow$

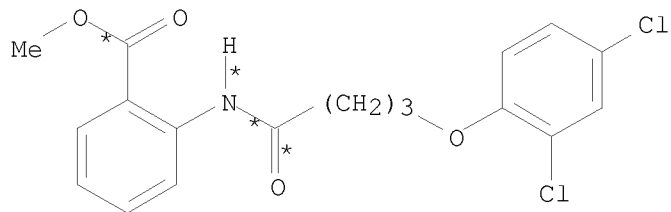


L

YIELD 88%

RX(5)      RCT    F 303794-61-8  
              RGT    J 302-01-2 N2H4  
              PRO    L 648859-11-4  
              SOL    71-36-3 BuOH  
              CON    8 - 10 hours, reflux

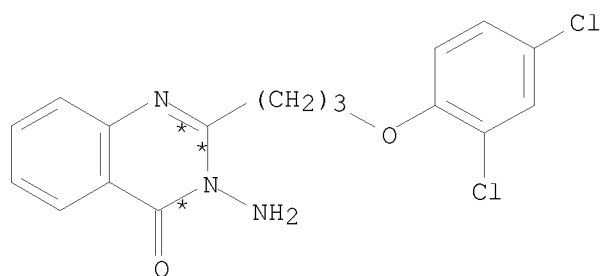
RX(6) OF 60      ...H ==> M...



H

(6)  $\longrightarrow$

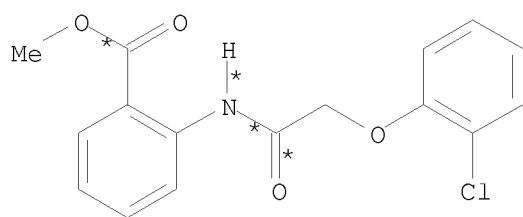
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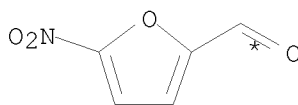
M  
YIELD 86%

RX(6)      RCT    H 346724-11-6  
               RGT    J 302-01-2 N2H4  
               PRO    M 1063716-16-4  
               SOL    71-36-3 BuOH  
               CON    8 - 10 hours, reflux

RX(26) OF 60 COMPOSED OF RX(4), RX(7)  
 RX(26)      C    +    N    ==>    O

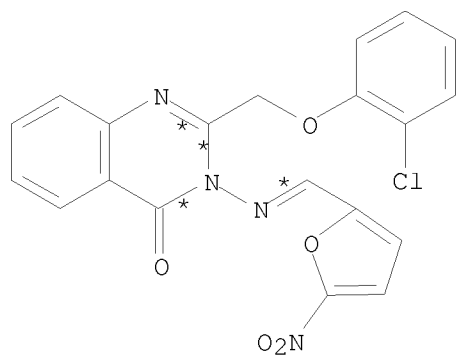


C



N

2  
STEPS  
→



O  
YIELD 70%

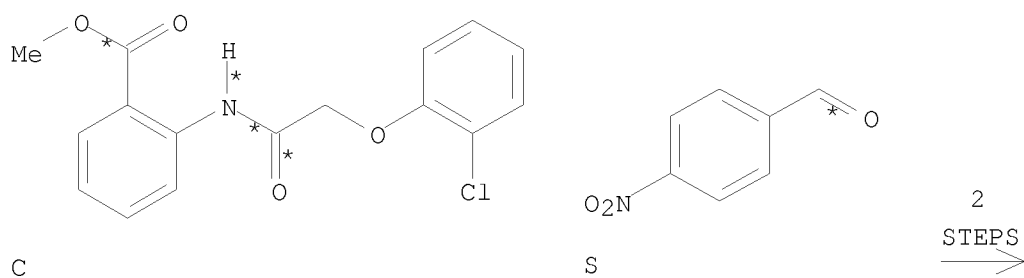
10/ 562,112

RX(4)      RCT   C 301678-87-5  
             RGT   J 302-01-2 N2H4  
             PRO   I 1063716-09-5  
             SOL   71-36-3 BuOH  
             CON   8 - 10 hours, reflux

RX(7)      RCT   I 1063716-09-5, N 698-63-5  
             PRO   O 1063716-20-0  
             SOL   64-19-7 AcOH  
             CON   4 hours, reflux  
             NTE   CHEMOSELECTIVE

RX(27) OF 60 COMPOSED OF RX(4), RX(10)

RX(27)      C + S ==> T



T  
YIELD 72%

RX(4)      RCT   C 301678-87-5  
             RGT   J 302-01-2 N2H4  
             PRO   I 1063716-09-5  
             SOL   71-36-3 BuOH  
             CON   8 - 10 hours, reflux

RX(10)      RCT   I 1063716-09-5, S 555-16-8  
             PRO   T 1063716-34-6  
             SOL   64-19-7 AcOH  
             CON   4 hours, reflux

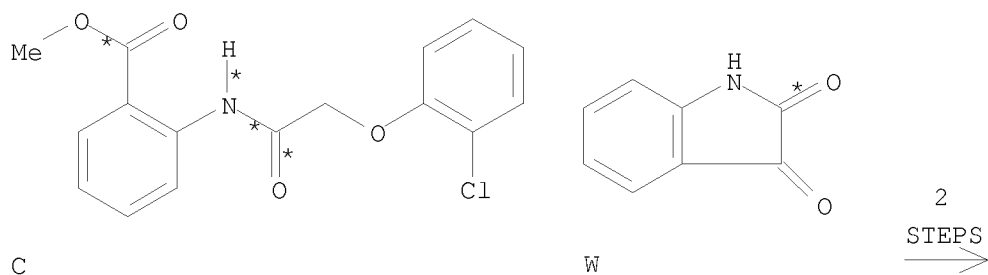


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NTE CHEMOSELECTIVE

RX(28) OF 60 COMPOSED OF RX(4), RX(13)

RX(28) C + W ==> X



X  
YIELD 75%

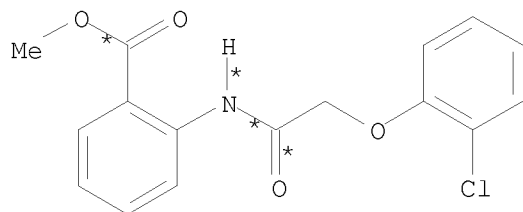
RX(4) RCT C 301678-87-5  
RGT J 302-01-2 N2H4  
PRO I 1063716-09-5  
SOL 71-36-3 BuOH  
CON 8 - 10 hours, reflux

RX(13) RCT I 1063716-09-5, W 91-56-5  
PRO X 1063716-48-2  
SOL 64-19-7 AcOH  
CON 4 - 6 hours, reflux

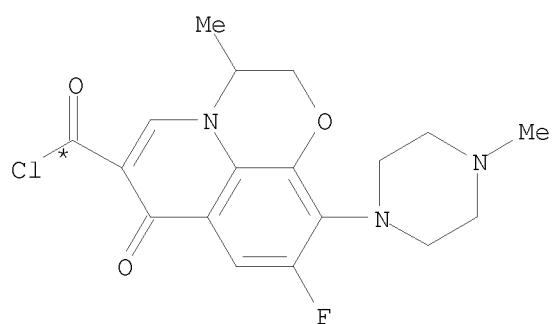
RX(29) OF 60 COMPOSED OF RX(4), RX(16)

RX(29) C + AA ==> AB

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C



AA

2  
STEPS  
→

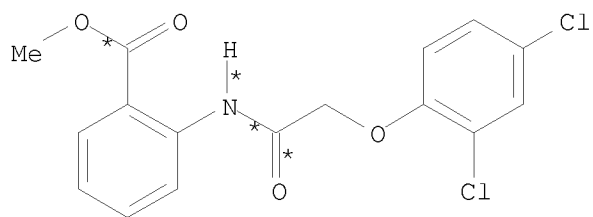
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(4)      RCT    C 301678-87-5  
          RGT    J 302-01-2 N2H4  
          PRO    I 1063716-09-5  
          SOL    71-36-3 BuOH  
          CON    8 - 10 hours, reflux

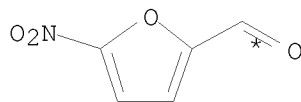
RX(16)     RCT    I 1063716-09-5, AA 784160-13-0  
          RGT    AC 584-08-7 K2CO3  
          PRO    AB 1063716-61-9  
          SOL    71-43-2 Benzene  
          CON    6 hours, reflux

RX(30) OF 60 COMPOSED OF RX(5), RX(8)  
RX(30)      F    +    N    ==>    Q

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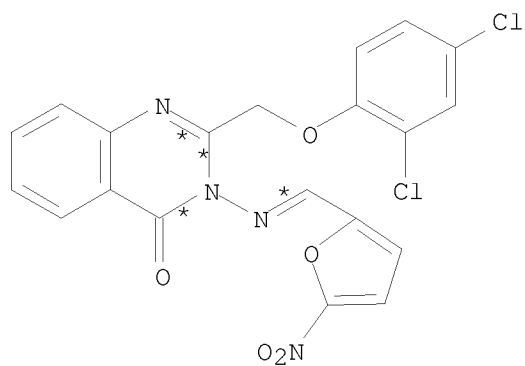


F



N

2  
STEPS  
→



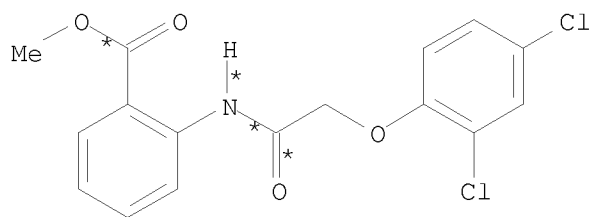
Q  
YIELD 73%

RX(5)      RCT    F 303794-61-8  
             RGT    J 302-01-2 N<sub>2</sub>H<sub>4</sub>  
             PRO    L 648859-11-4  
             SOL    71-36-3 BuOH  
             CON    8 - 10 hours, reflux

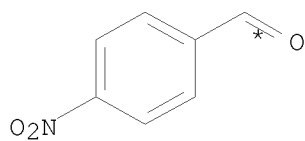
RX(8)      RCT    L 648859-11-4, N 698-63-5  
             PRO    Q 1063716-24-4  
             SOL    64-19-7 AcOH  
             CON    4 hours, reflux  
             NTE    CHEMOSELECTIVE

RX(31) OF 60 COMPOSED OF RX(5), RX(11)  
RX(31)      F    +    S    ==>    U

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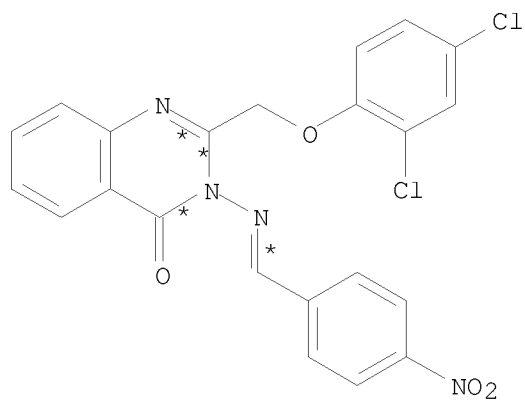


F



S

2  
STEPS  
→



U

YIELD 72%

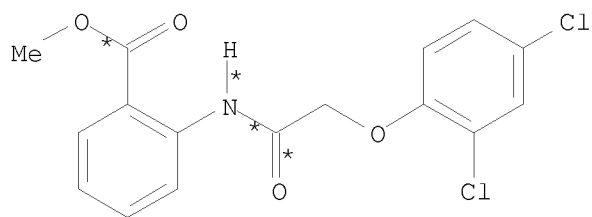
RX(5)      RCT    F 303794-61-8  
             RGT    J 302-01-2 N<sub>2</sub>H<sub>4</sub>  
             PRO    L 648859-11-4  
             SOL    71-36-3 BuOH  
             CON    8 - 10 hours, reflux

RX(11)     RCT    L 648859-11-4, S 555-16-8  
             PRO    U 1063716-40-4  
             SOL    64-19-7 AcOH  
             CON    4 hours, reflux  
             NTE    CHEMOSELECTIVE

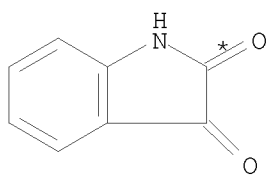
RX(32) OF 60 COMPOSED OF RX(5), RX(14)

RX(32)      F    +    W    ==>    Y

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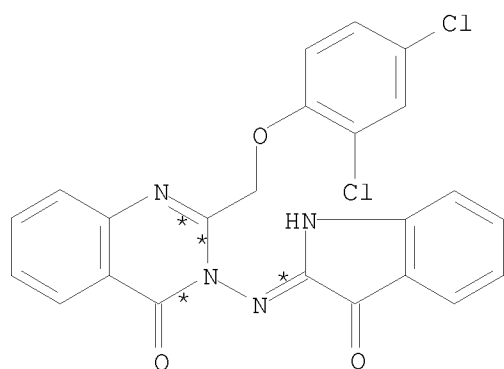


F



W

2  
STEPS  
→

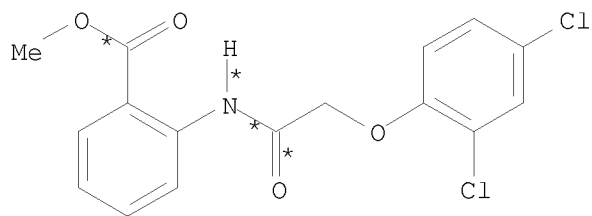


Y  
YIELD 72%

RX(5)      RCT    F 303794-61-8  
            RGT    J 302-01-2 N2H4  
            PRO    L 648859-11-4  
            SOL    71-36-3 BuOH  
            CON    8 - 10 hours, reflux

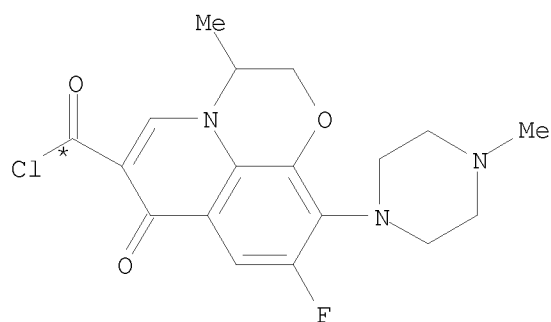
RX(14)     RCT    L 648859-11-4, W 91-56-5  
            PRO    Y 1063716-53-9  
            SOL    64-19-7 AcOH  
            CON    4 - 6 hours, reflux

RX(33) OF 60 COMPOSED OF RX(5), RX(17)  
RX(33)      F    +    AA    ==>    AE



F

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AA

2  
STEPS  
→

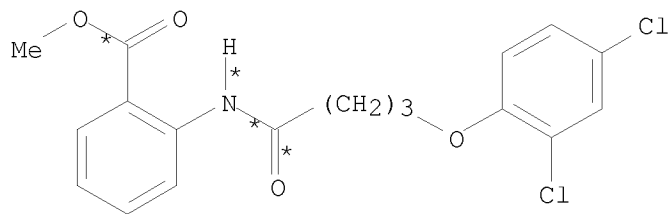
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(5) RCT F 303794-61-8  
RGT J 302-01-2 N2H4  
PRO L 648859-11-4  
SOL 71-36-3 BuOH  
CON 8 - 10 hours, reflux

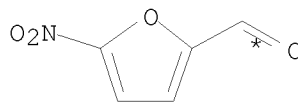
RX(17) RCT L 648859-11-4, AA 784160-13-0  
RGT AC 584-08-7 K2CO3  
PRO AE 1063716-64-2  
SOL 71-43-2 Benzene  
CON 6 hours, reflux

RX(34) OF 60 COMPOSED OF RX(6), RX(9)

RX(34) H + N ==> R



H

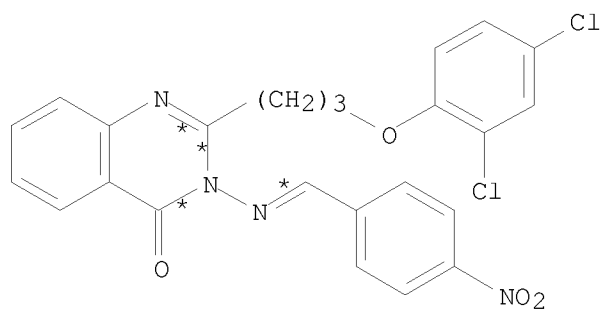


N

2  
STEPS  
→



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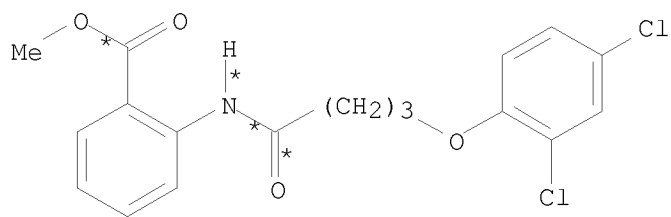


V  
YIELD 75%

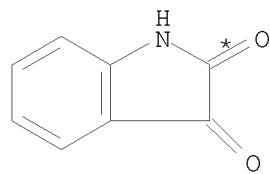
RX(6) RCT H 346724-11-6  
RGT J 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO M 1063716-16-4  
SOL 71-36-3 BuOH  
CON 8 - 10 hours, reflux

RX(12) RCT M 1063716-16-4, S 555-16-8  
PRO V 1063716-43-7  
SOL 64-19-7 AcOH  
CON 4 hours, reflux  
NTE CHEMOSELECTIVE

RX(36) OF 60 COMPOSED OF RX(6), RX(15)  
RX(36) H + W ==> Z



H

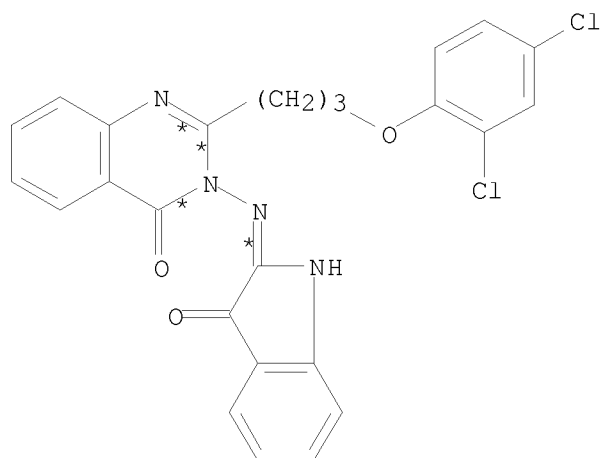


W

2  
STEPS  
→



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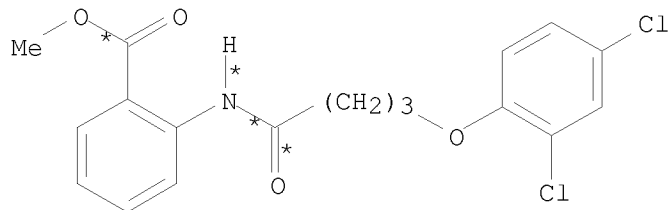


Z  
YIELD 70%

RX(6)      RCT    H 346724-11-6  
              RGT    J 302-01-2 N2H4  
              PRO    M 1063716-16-4  
              SOL    71-36-3 BuOH  
              CON    8 - 10 hours, reflux

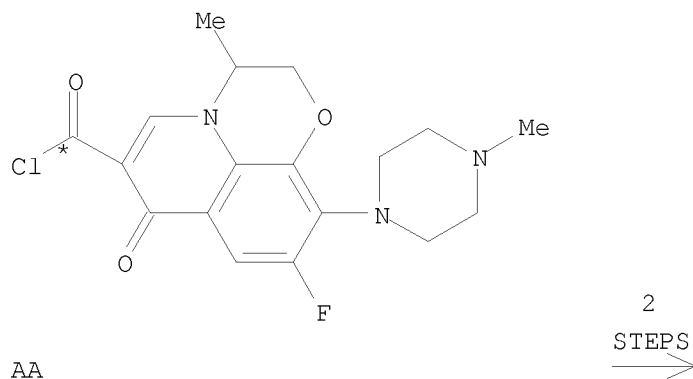
RX(15)      RCT    M 1063716-16-4, W 91-56-5  
              PRO    Z 1063716-57-3  
              SOL    64-19-7 AcOH  
              CON    4 - 6 hours, reflux

RX(37) OF 60 COMPOSED OF RX(6), RX(18)  
 RX(37)      H    +    AA    ==>    AF



H

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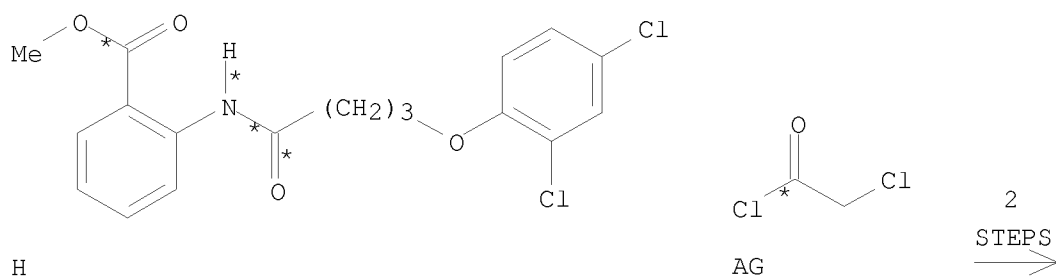


\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

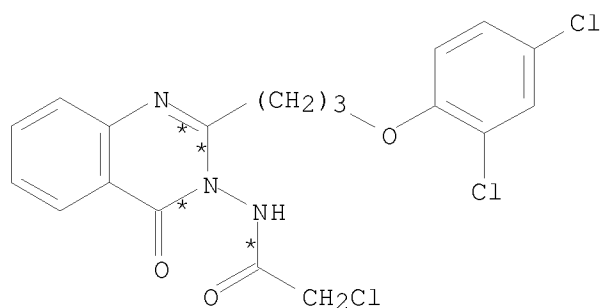
RX(6) RCT H 346724-11-6  
RGT J 302-01-2 N2H4  
PRO M 1063716-16-4  
SOL 71-36-3 BuOH  
CON 8 - 10 hours, reflux

RX(18) RCT M 1063716-16-4, AA 784160-13-0  
RGT AC 584-08-7 K2CO3  
PRO AF 1063716-67-5  
SOL 71-43-2 Benzene  
CON 6 hours, reflux

RX(38) OF 60 COMPOSED OF RX(6), RX(19)  
RX(38) H + AG ==> AH



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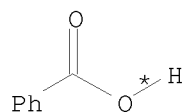
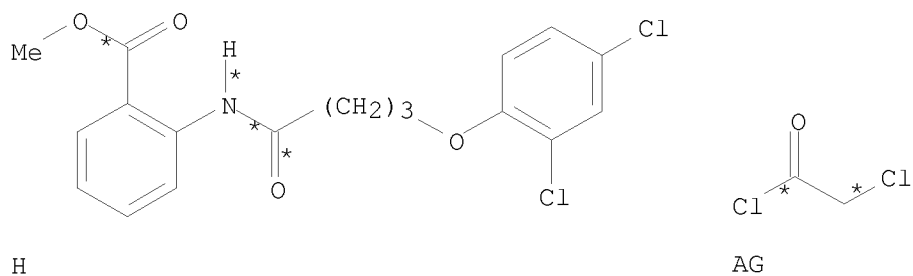


AH  
YIELD 80%

RX(6)      RCT    H 346724-11-6  
             RGT    J 302-01-2 N2H4  
             PRO    M 1063716-16-4  
             SOL    71-36-3 BuOH  
             CON    8 - 10 hours, reflux

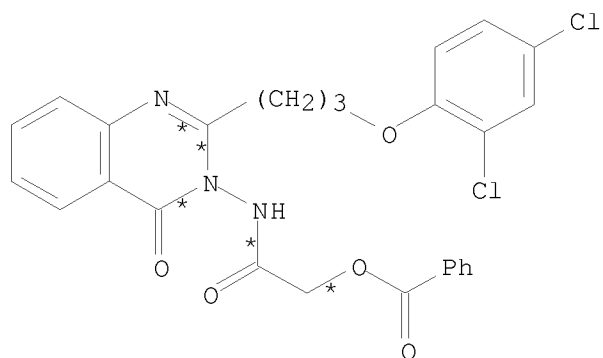
RX(19)     RCT    M 1063716-16-4, AG 79-04-9  
             PRO    AH 1063716-70-0  
             SOL    68-12-2 DMF  
             CON    SUBSTAGE(1) room temperature  
                     SUBSTAGE(2) 2 - 3 hours, room temperature

RX(55) OF 60 COMPOSED OF RX(6), RX(19), RX(20)  
RX(55)      H    +    AG    +    AJ    ==>    AK



● K  
AJ                      3  
                     STEPS  
                     →

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AK

YIELD 75%

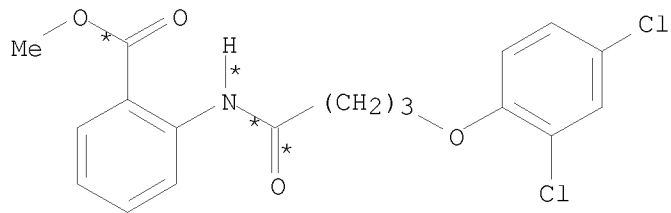
RX(6) RCT H 346724-11-6  
RGT J 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO M 1063716-16-4  
SOL 71-36-3 BuOH  
CON 8 - 10 hours, reflux

RX(19) RCT M 1063716-16-4, AG 79-04-9  
PRO AH 1063716-70-0  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 2 - 3 hours, room temperature

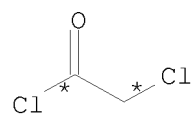
RX(20) RCT AH 1063716-70-0, AJ 582-25-2  
PRO AK 1063716-72-2  
SOL 68-12-2 DMF  
CON 4 - 6 hours, heated

RX(56) OF 60 COMPOSED OF RX(6), RX(19), RX(21)

RX(56) H + AG + AL ==> AM

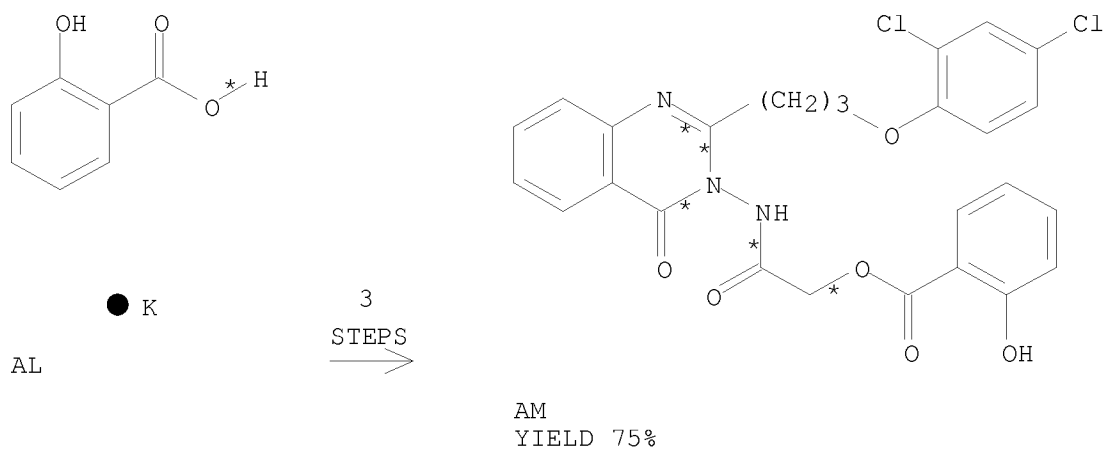


H



AG

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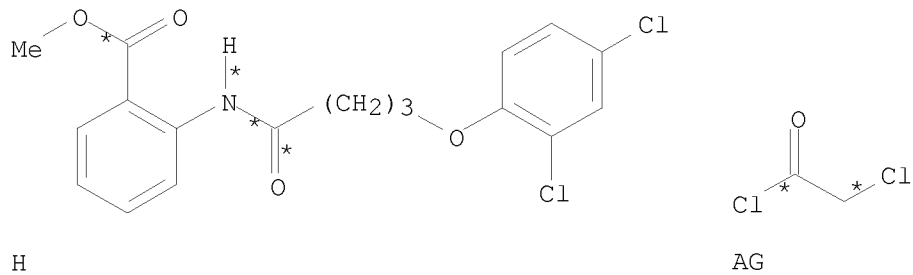


RX(6) RCT H 346724-11-6  
RGT J 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO M 1063716-16-4  
SOL 71-36-3 BuOH  
CON 8 - 10 hours, reflux

RX(19) RCT M 1063716-16-4, AG 79-04-9  
PRO AH 1063716-70-0  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 2 - 3 hours, room temperature

RX(21) RCT AH 1063716-70-0, AL 578-36-9  
PRO AM 1063716-76-6  
SOL 68-12-2 DMF  
CON 4 - 6 hours, heated

RX(57) OF 60 COMPOSED OF RX(6), RX(19), RX(22)  
RX(57) H + AG + AN ==> AO

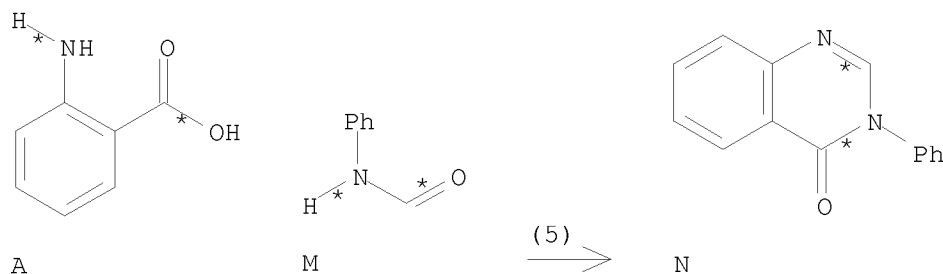




REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 149:245729 CASREACT  
 TITLE: Anthranilic Acid  
 AUTHOR(S): Castedo, Luis; Guitian, Enrique  
 CORPORATE SOURCE: Spain  
 SOURCE: e-EROS Encyclopedia of Reagents for Organic Synthesis (2001), No pp. given. John Wiley & Sons, Ltd.: Chichester, UK.  
 CODEN: 69KUHI  
 URL: <http://www3.interscience.wiley.com/cgi-bin/mrwhome/104554785/HOME>  
 DOCUMENT TYPE: Conference; General Review; (online computer file)  
 LANGUAGE: English  
 AB A review of the article Anthranilic Acid.

RX(5) OF 5 A + M ==> N



RX(5) RCT A 118-92-3, M 103-70-8  
 PRO N 16347-60-7  
 CON 130 deg C  
 NTE Synthesis of Heterocycles

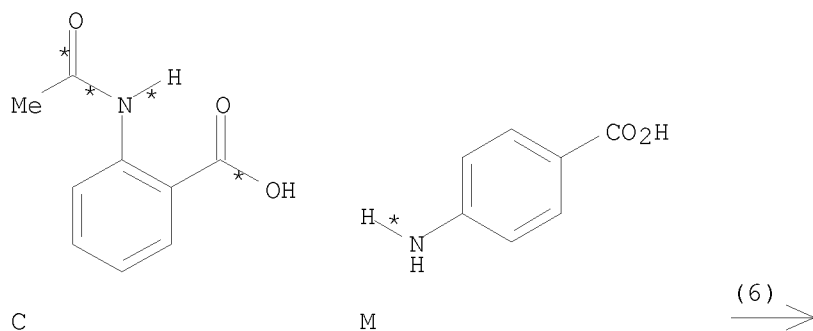
L3 ANSWER 3 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 148:538299 CASREACT  
 TITLE: Process for synthesis of quinazolinones as antimycobacterial agents  
 INVENTOR(S): Meyyanathan, S. N.; Suresh, Bhojraj; Anbunathan, Perumal Nirmala  
 PATENT ASSIGNEE(S): India  
 SOURCE: Indian Pat. Appl., 14pp.  
 CODEN: INXXBQ  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 2004CH01048	A	20070309	IN 2004-CH1048	20041011
PRIORITY APPLN. INFO.:			IN 2004-CH1048	20041011

OTHER SOURCE(S): MARPAT 148:538299

AB A process for the synthesis of 4-(2-methyl-4-oxo-4h-quinazolin-3-yl)-benzoyl pyrrolidine-2-carboxylic acid starting from anthranilic acids and acetic anhydride. The claimed compds. are active against Mycobacterium tuberculosis.

RX(6) OF 44 ...C + M ==&gt; N...



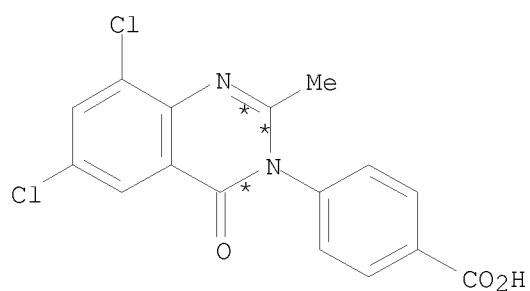
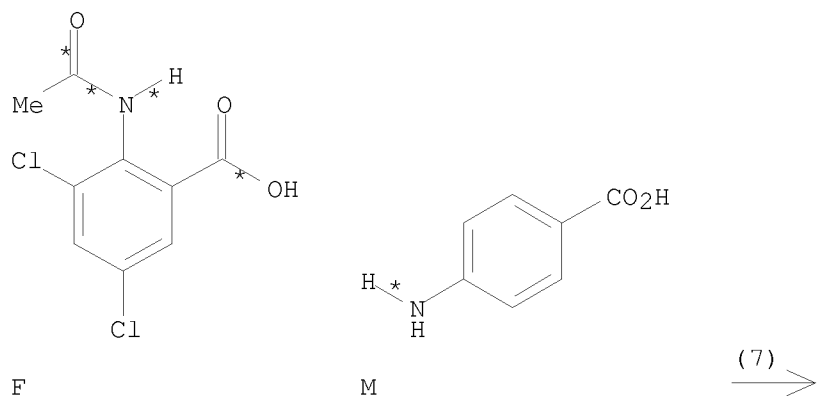
N  
YIELD 93%

RX(6) RCT C 89-52-1, M 150-13-0  
 RGT O 64-19-7 AcOH, P 1314-56-3 P205  
 PRO N 4005-05-4  
 SOL 7732-18-5 Water  
 CON 6 hours, reflux

RX(7) OF 44 ...F + M ==&gt; R...



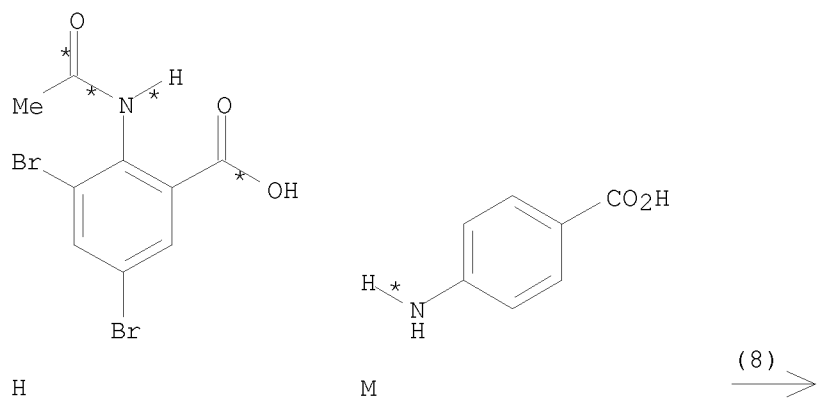
10/ 562,112



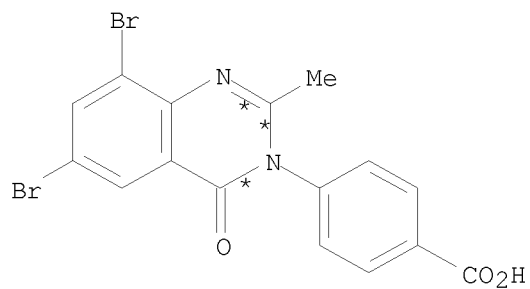
R  
YIELD 89%

RX(7)      RCT   F 19094-64-5, M 150-13-0  
              RGT   O 64-19-7 AcOH, P 1314-56-3 P205  
              PRO   R 1023888-34-7  
              SOL   7732-18-5 Water  
              CON   8.5 hours, reflux

RX(8) OF 44      ...H + M ==> S...



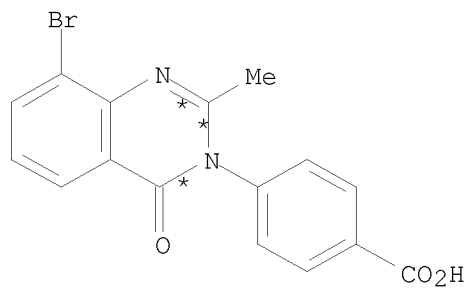
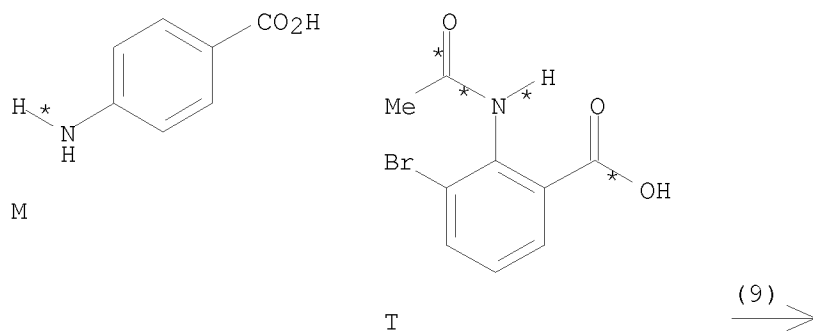
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S  
YIELD 100%

RX(8)        RCT   H 16610-45-0, M 150-13-0  
              RGT   O 64-19-7 AcOH, P 1314-56-3 P205  
              PRO   S 24295-52-1  
              SOL   7732-18-5 Water  
              CON   5.5 hours, reflux

RX(9) OF 44        M   +   T   ==>   U...

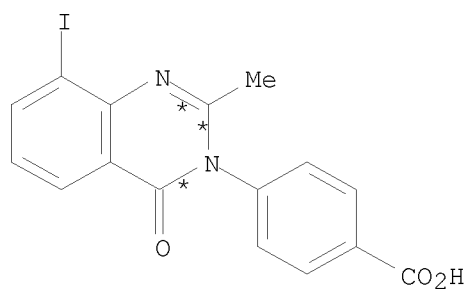
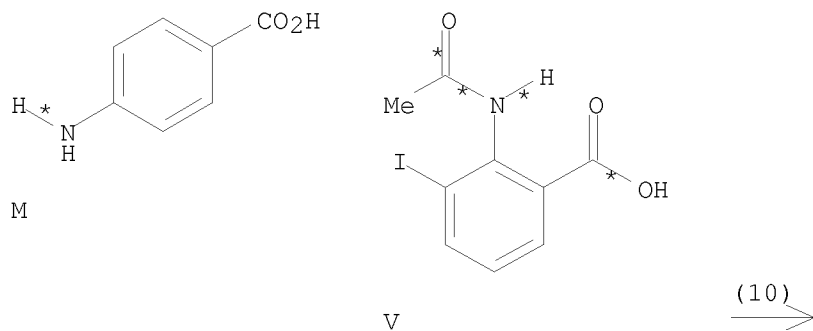


U  
YIELD 93%

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RX(9)        RCT   M 150-13-0, T 861791-77-7  
              RGT   O 64-19-7 AcOH, P 1314-56-3 P2O5  
              PRO   U 1023888-35-8  
              SOL   7732-18-5 Water  
              CON   5.5 hours, reflux

RX(10) OF 44        M   +   V   ==>   W...

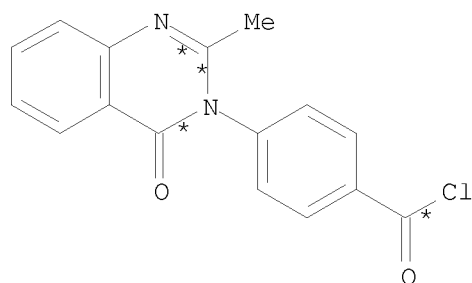
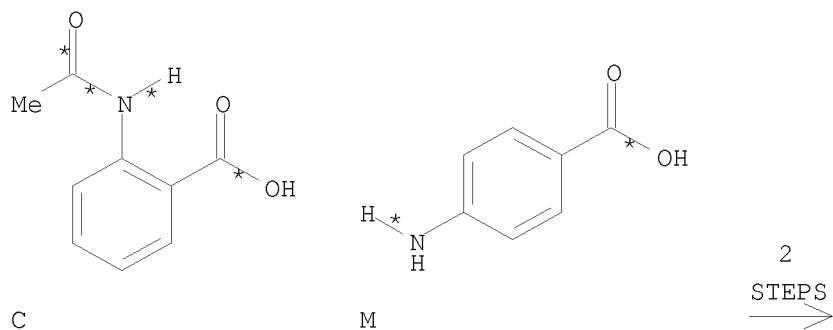


W  
YIELD 100%

RX(10)        RCT   M 150-13-0, V 1027340-18-6  
              RGT   O 64-19-7 AcOH, P 1314-56-3 P2O5  
              PRO   W 1023888-36-9  
              SOL   7732-18-5 Water  
              CON   3 hours, reflux

RX(24) OF 44 COMPOSED OF RX(6), RX(11)  
RX(24)        C   +   M   ==>   X

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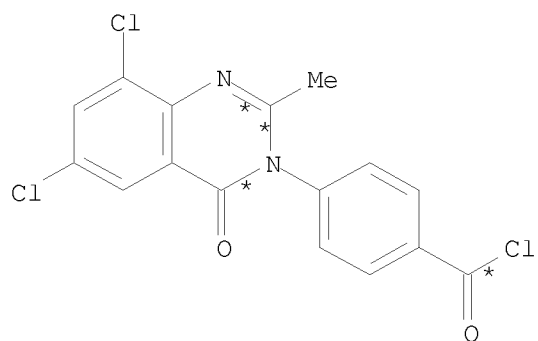
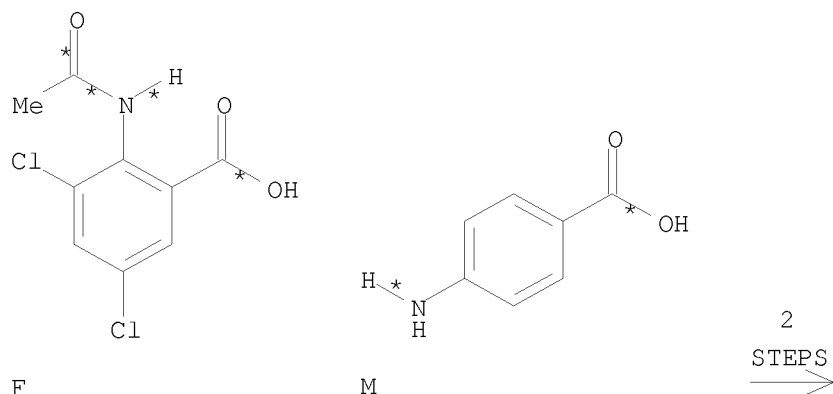
X  
YIELD 85%

RX(6) RCT C 89-52-1, M 150-13-0  
RGT O 64-19-7 AcOH, P 1314-56-3 P205  
PRO N 4005-05-4  
SOL 7732-18-5 Water  
CON 6 hours, reflux

RX(11) RCT N 4005-05-4  
RGT Y 7719-09-7 SOCl<sub>2</sub>  
PRO X 863988-62-9  
SOL 123-91-1 Dioxane  
CON 4 hours, reflux

RX(25) OF 44 COMPOSED OF RX(7), RX(12)  
RX(25) F + M ==> AA

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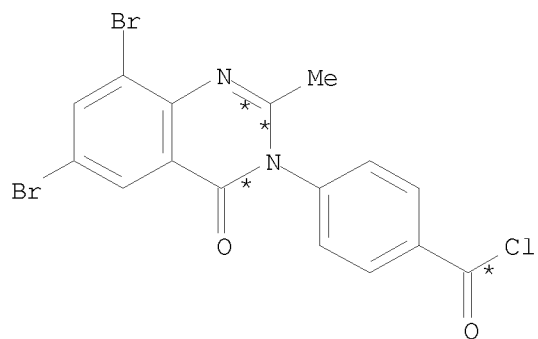
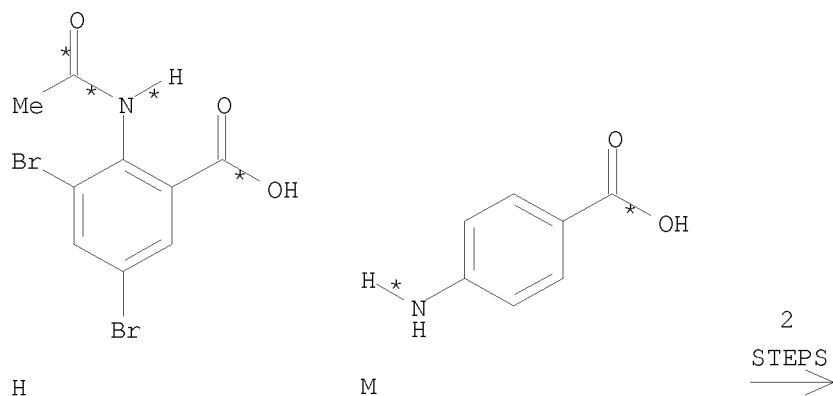
AA  
YIELD 82%

RX(7) RCT F 19094-64-5, M 150-13-0  
RGT O 64-19-7 AcOH, P 1314-56-3 P2O5  
PRO R 1023888-34-7  
SOL 7732-18-5 Water  
CON 8.5 hours, reflux

RX(12) RCT R 1023888-34-7  
RGT Y 7719-09-7 SOCl2  
PRO AA 1023888-37-0  
SOL 123-91-1 Dioxane  
CON 6 hours, reflux

RX(26) OF 44 COMPOSED OF RX(8), RX(13)  
RX(26) H + M ==> AB

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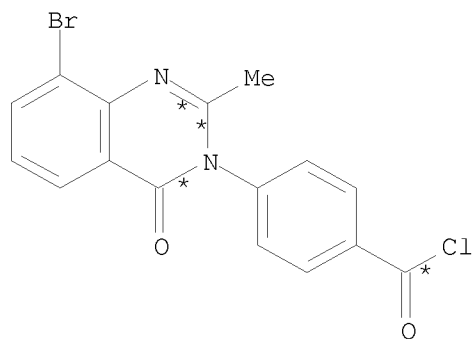
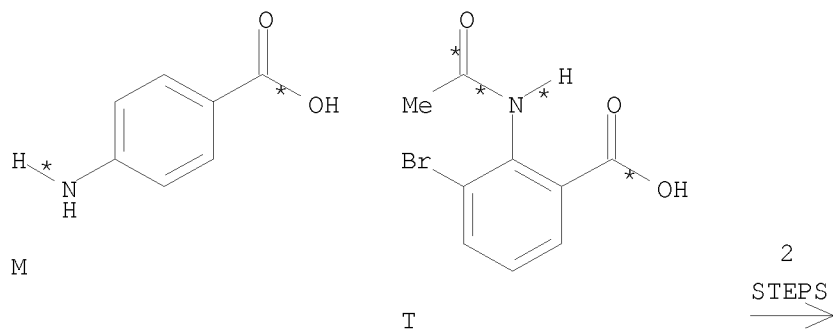
AB  
YIELD 77%

RX(8) RCT H 16610-45-0, M 150-13-0  
RGT O 64-19-7 AcOH, P 1314-56-3 P2O5  
PRO S 24295-52-1  
SOL 7732-18-5 Water  
CON 5.5 hours, reflux

RX(13) RCT S 24295-52-1  
RGT Y 7719-09-7 SOCl2  
PRO AB 1023888-38-1  
SOL 123-91-1 Dioxane  
CON 6.25 hours, reflux

RX(27) OF 44 COMPOSED OF RX(9), RX(14)  
RX(27) M + T ==> AC

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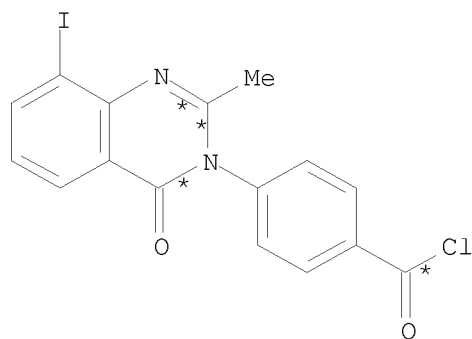
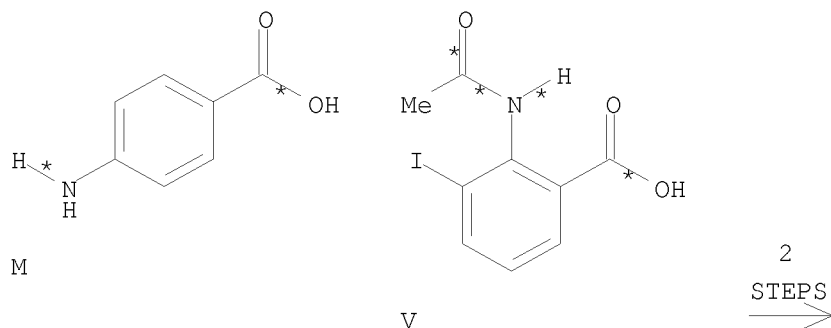
AC  
YIELD 97%

RX(9) RCT M 150-13-0, T 861791-77-7  
RGT O 64-19-7 AcOH, P 1314-56-3 P205  
PRO U 1023888-35-8  
SOL 7732-18-5 Water  
CON 5.5 hours, reflux

RX(14) RCT U 1023888-35-8  
RGT Y 7719-09-7 SOCl2  
PRO AC 1023888-39-2  
SOL 123-91-1 Dioxane  
CON 10 hours, reflux

RX(28) OF 44 COMPOSED OF RX(10), RX(15)  
RX(28) M + V ==> AD

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AD  
YIELD 60%

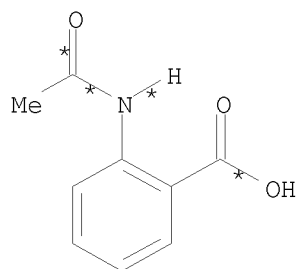
RX(10) RCT M 150-13-0, V 1027340-18-6  
RGT O 64-19-7 AcOH, P 1314-56-3 P205  
PRO W 1023888-36-9  
SOL 7732-18-5 Water  
CON 3 hours, reflux

RX(15) RCT W 1023888-36-9  
RGT Y 7719-09-7 SOCl<sub>2</sub>  
PRO AD 1023888-40-5  
SOL 123-91-1 Dioxane  
CON 7.5 hours, reflux

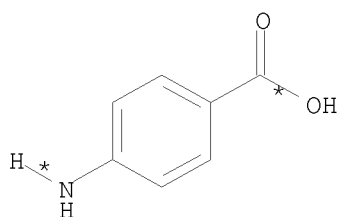
RX(37) OF 44 COMPOSED OF RX(6), RX(11), RX(16)  
RX(37) C + M + AE ==> AF



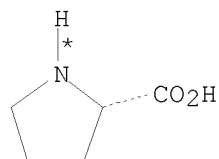
10/ 562,112



C

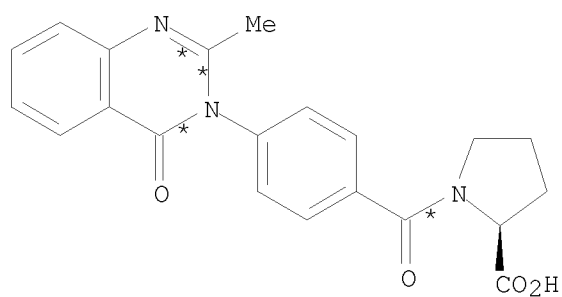


M



AE

3  
STEPS  
→

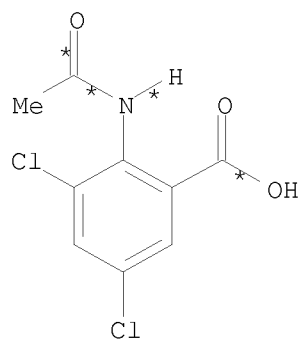


AF  
YIELD 66%

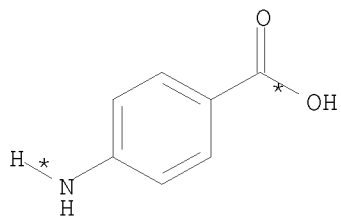
RX(6)	RCT	C 89-52-1, M 150-13-0
	RGT	O 64-19-7 AcOH, P 1314-56-3 P205
	PRO	N 4005-05-4
	SOL	7732-18-5 Water
	CON	6 hours, reflux
RX(11)	RCT	N 4005-05-4
	RGT	Y 7719-09-7 SOCl <sub>2</sub>
	PRO	X 863988-62-9
	SOL	123-91-1 Dioxane
	CON	4 hours, reflux
RX(16)	RCT	X 863988-62-9, AE 147-85-3
	RGT	AG 1310-73-2 NaOH
	PRO	AF 1023888-41-6
	SOL	7732-18-5 Water, 123-91-1 Dioxane
	CON	6 hours, reflux

RX(39) OF 44 COMPOSED OF RX(7), RX(12), RX(17)  
RX(39) F + M + AE ==> AH

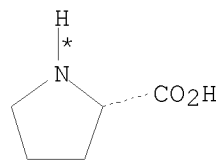
10/ 562,112



F

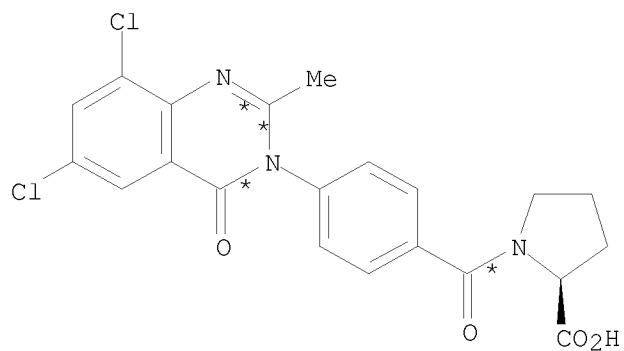


M



AE

3  
STEPS  
→

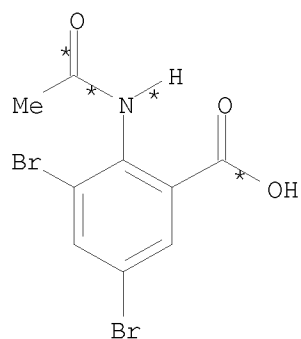


AH  
YIELD 63%

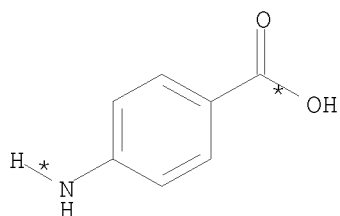
RX(7)	RCT	F 19094-64-5, M 150-13-0
	RGT	O 64-19-7 AcOH, P 1314-56-3 P205
	PRO	R 1023888-34-7
	SOL	7732-18-5 Water
	CON	8.5 hours, reflux
RX(12)	RCT	R 1023888-34-7
	RGT	Y 7719-09-7 SOCl2
	PRO	AA 1023888-37-0
	SOL	123-91-1 Dioxane
	CON	6 hours, reflux
RX(17)	RCT	AA 1023888-37-0, AE 147-85-3
	RGT	AG 1310-73-2 NaOH
	PRO	AH 1023888-42-7
	SOL	7732-18-5 Water, 123-91-1 Dioxane
	CON	10.25 hours, reflux

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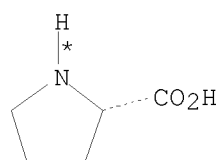
RX(41) OF 44 COMPOSED OF RX(8), RX(13), RX(18)  
RX(41) H + M + AE ==> AI



H

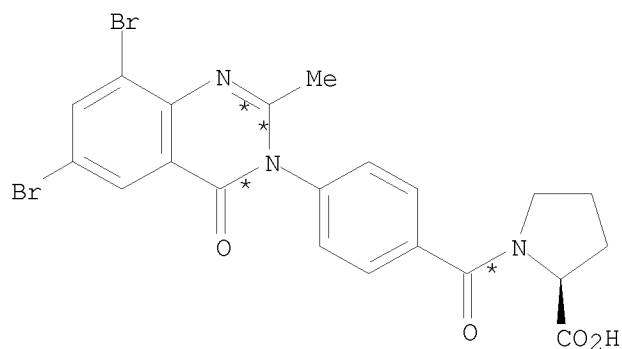


M



AE

3  
STEPS  
→



AI  
YIELD 88%

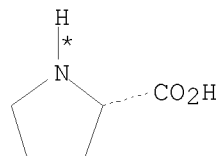
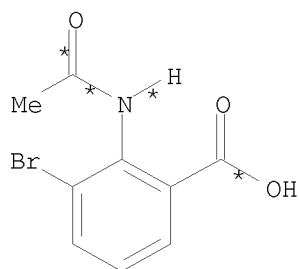
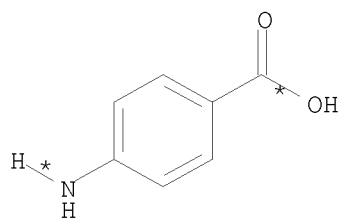
RX(8)	RCT	H 16610-45-0, M 150-13-0
	RGT	O 64-19-7 AcOH, P 1314-56-3 P205
	PRO	S 24295-52-1
	SOL	7732-18-5 Water
	CON	5.5 hours, reflux
RX(13)	RCT	S 24295-52-1
	RGT	Y 7719-09-7 SOCl2
	PRO	AB 1023888-38-1
	SOL	123-91-1 Dioxane
	CON	6.25 hours, reflux
RX(18)	RCT	AB 1023888-38-1, AE 147-85-3
	RGT	AG 1310-73-2 NaOH
	PRO	AI 1023888-43-8
	SOL	7732-18-5 Water, 123-91-1 Dioxane

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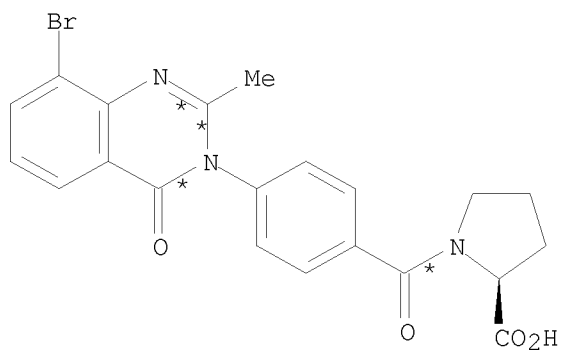
CON 8 hours, reflux

RX(43) OF 44 COMPOSED OF RX(9), RX(14), RX(19)

RX(43) M + T + AE ==> AJ



3  
STEPS  
→



AJ  
YIELD 86%

RX(9) RCT M 150-13-0, T 861791-77-7  
RGT O 64-19-7 AcOH, P 1314-56-3 P205  
PRO U 1023888-35-8  
SOL 7732-18-5 Water  
CON 5.5 hours, reflux

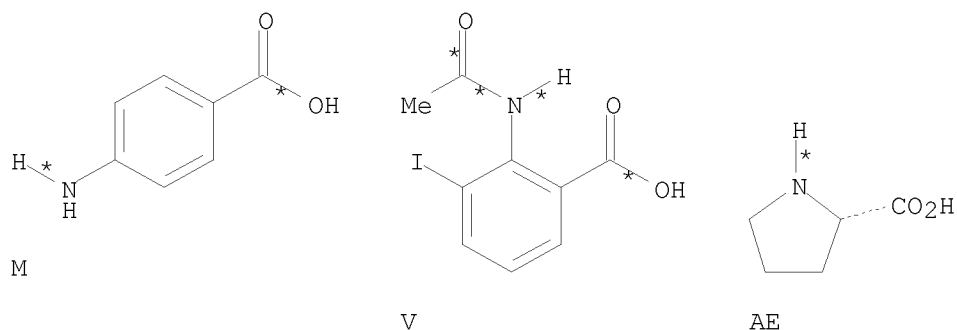
RX(14) RCT U 1023888-35-8  
RGT Y 7719-09-7 SOCl2  
PRO AC 1023888-39-2  
SOL 123-91-1 Dioxane  
CON 10 hours, reflux

RX(19) RCT AC 1023888-39-2, AE 147-85-3  
RGT AG 1310-73-2 NaOH  
PRO AJ 1023888-44-9

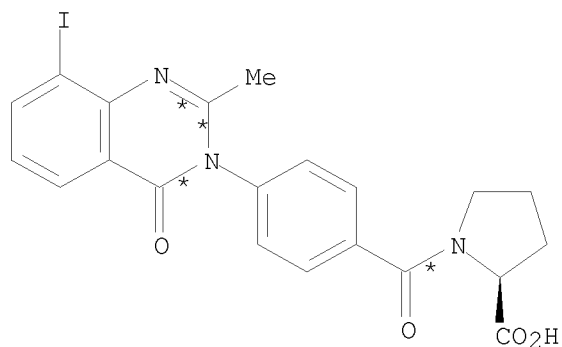
10/ 562,112

SOL 7732-18-5 Water, 123-91-1 Dioxane  
CON 8 hours, reflux

RX(44) OF 44 COMPOSED OF RX(10), RX(15), RX(20)  
RX(44) M + V + AE ==> AK



3  
STEPS  
=>



AK  
YIELD 57%

RX(10) RCT M 150-13-0, V 1027340-18-6  
RGT O 64-19-7 AcOH, P 1314-56-3 P205  
PRO W 1023888-36-9  
SOL 7732-18-5 Water  
CON 3 hours, reflux

RX(15) RCT W 1023888-36-9  
RGT Y 7719-09-7 SOCl2  
PRO AD 1023888-40-5  
SOL 123-91-1 Dioxane  
CON 7.5 hours, reflux

RX(20) RCT AD 1023888-40-5, AE 147-85-3  
RGT AG 1310-73-2 NaOH

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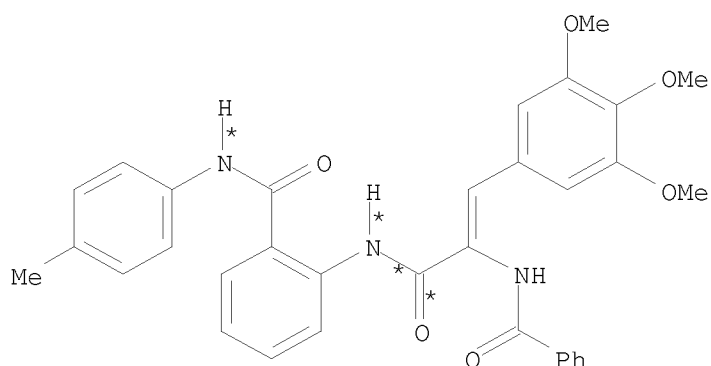
PRO AK 1023888-45-0  
SOL 7732-18-5 Water, 123-91-1 Dioxane  
CON 10.75 hours, reflux

L3 ANSWER 4 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 148:495870 CASREACT  
TITLE: Synthesis of new thiadiazoles,  
1,2,4-triazolo[3,4-b]-1,3,4-thiadiazoles, and  
1,2,4-triazolo[2,3-c]quinazoline derivatives from  
4H-3,1-benzoxazin-4-one derivative  
AUTHOR(S): Mahmoud, M. R.; El-Bordany, E. A.; Azab, M. E.;  
Soliman, E. A.  
CORPORATE SOURCE: Chemistry Department, Ain Shams University, Cairo,  
Egypt  
SOURCE: Phosphorus, Sulfur and Silicon and the Related  
Elements (2007), 182(6), 1275-1289  
CODEN: PSSLEC; ISSN: 1042-6507  
PUBLISHER: Taylor & Francis, Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB 4H-3,1-benzoxazin-4-one derivative (I) was reacted with Grignard reagents,  
primary and secondary amines, glycine, hydrazine hydrate, azines, and a  
Schiff base. The acid hydrazide derivative (II) was the key starting material  
for the synthesis of triazole, triazolo[3,4-b]thiadiazole, thiadiazole,  
and triazolo[2,3-c]quinazoline derivs., e.g., III and IV.

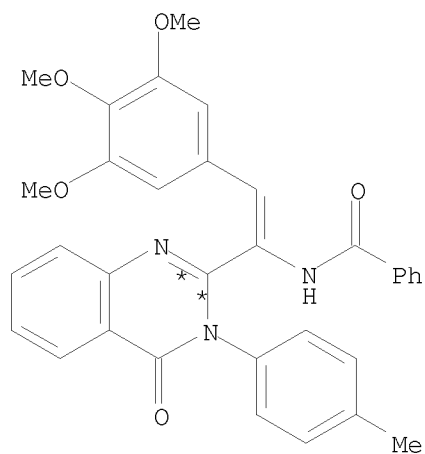
RX(24) OF 69 ...AY ==> BB



AY

(24)

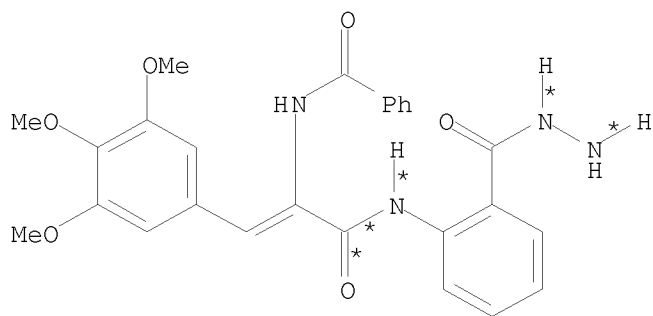
10/ 562,112



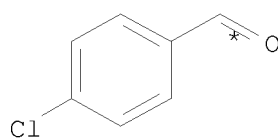
BB  
YIELD 70%

RX(24)     RCT    AY 1020730-48-6  
             PRO    BB 1020730-49-7  
             CON    SUBSTAGE(1) 1 hour, 200 deg C  
                      SUBSTAGE(2) cooled

RX(26) OF 69     ...AE   +   BD   ==>   BE



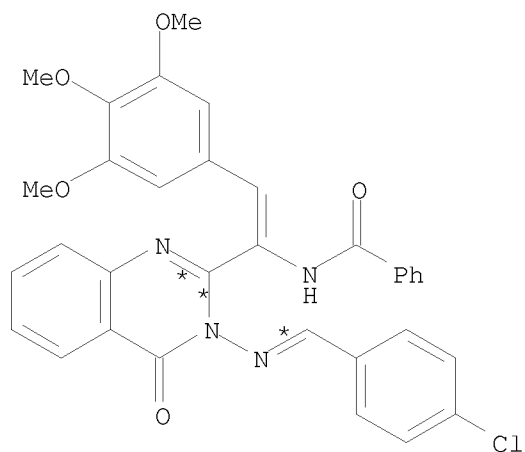
AE



BD

(26)  
→

10/ 562,112



BE

RX(26) RCT AE 1020730-27-1, BD 104-88-1  
RGT BC 127-09-3 AcONa  
PRO BE 1020730-50-0  
SOL 64-19-7 AcOH  
CON 3 hours, reflux

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

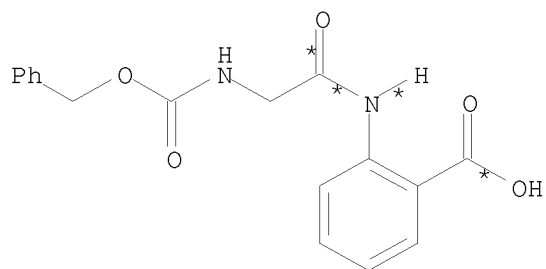
L3 ANSWER 5 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 148:417239 CASREACT  
TITLE: Potent Inhibitors of the Hedgehog Signaling Pathway  
AUTHOR(S): Brunton, Shirley A.; Stibbard, John H. A.; Rubin, Lee L.; Kruse, Lawrence I.; Guicherit, Oivin M.; Boyd, Edward A.; Price, Steven  
CORPORATE SOURCE: Evotec, Abingdon, Oxfordshire, OX14 4RX, UK  
SOURCE: Journal of Medicinal Chemistry (2008), 51(5), 1108-1110  
CODEN: JMCMAR; ISSN: 0022-2623  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB A small family of Ph quinazolinone ureas is reported as potent modulators of Hedgehog protein function. Preliminary SAR studies of the urea substituent led to a nanomolar Hedgehog antagonist.

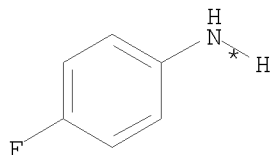
RX(12) OF 105 ...AG + AJ ==> AK...



10/ 562,112

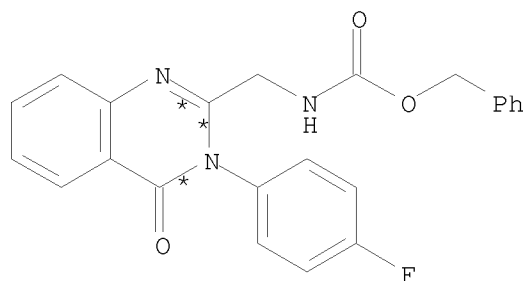


AG



AJ

(12)  $\longrightarrow$



AK

YIELD 48%

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone

SOL 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4

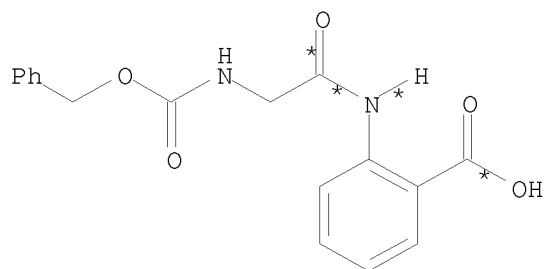
SOL 109-99-9 THF

CON 20 hours, room temperature -> 70 deg C

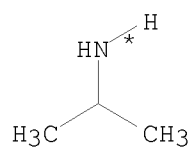
PRO AK 330796-22-0

RX(27) OF 105 ...AG + BQ ==> BP...

10/ 562,112

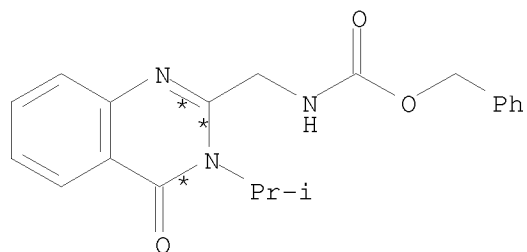


AG



BQ

(27) →

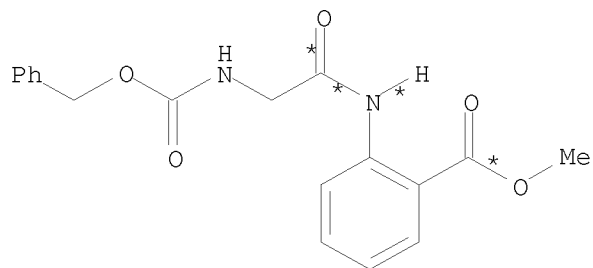


BP

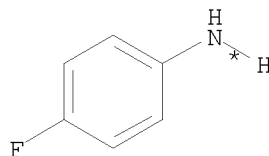
YIELD 48%

RX(27) RCT AG 55301-19-4, BQ 75-31-0  
 RGT AE 530-62-1 Diimidazolyl ketone  
 PRO BP 1072784-96-3  
 SOL 109-99-9 THF  
 CON 20 hours, reflux

RX(35) OF 105 COMPOSED OF RX(11), RX(12)  
 RX(35) AD + AJ ==> AK



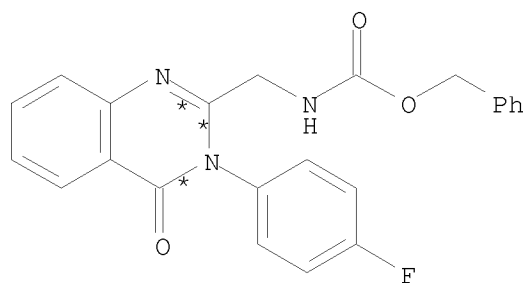
AD



AJ

2  
 STEPS  
 →

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AK  
YIELD 48%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH

SOL 7732-18-5 Water, 123-91-1 Dioxane

CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

CON pH 1

PRO AG 55301-19-4

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone

SOL 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4

SOL 109-99-9 THF

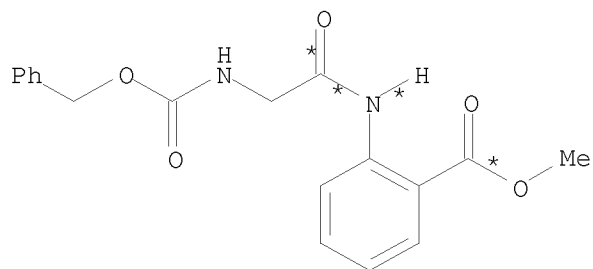
CON 20 hours, room temperature -> 70 deg C

PRO AK 330796-22-0

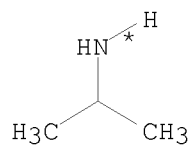
RX(36) OF 105 COMPOSED OF RX(11), RX(27)

RX(36) AD + BQ ==> BP

10/ 562,112

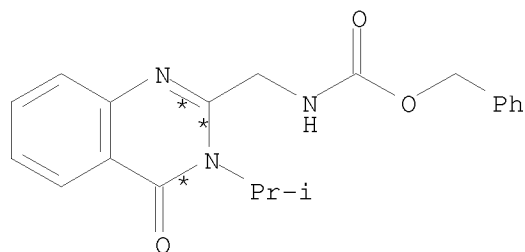


AD



BQ

2  
STEPS  
→



BP

YIELD 48%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH

SOL 7732-18-5 Water, 123-91-1 Dioxane

CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

CON pH 1

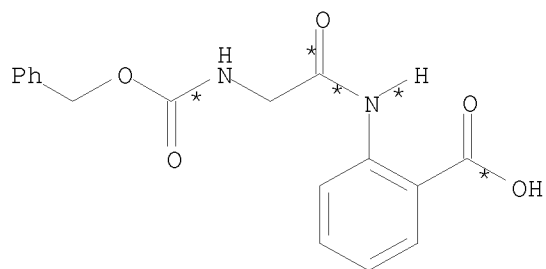
PRO AG 55301-19-4

RX(27) RCT AG 55301-19-4, BQ 75-31-0  
RGT AE 530-62-1 Diimidazolyl ketone  
PRO BP 1072784-96-3  
SOL 109-99-9 THF  
CON 20 hours, reflux

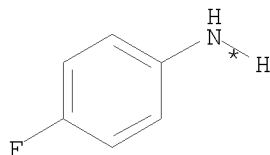
RX(37) OF 105 COMPOSED OF RX(12), RX(13)

RX(37) AG + AJ ==> AL

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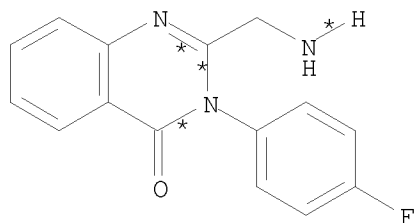


AG



AJ

2  
STEPS  
→



AL  
YIELD 95%

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone

SOL 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4

SOL 109-99-9 THF

CON 20 hours, room temperature -> 70 deg C

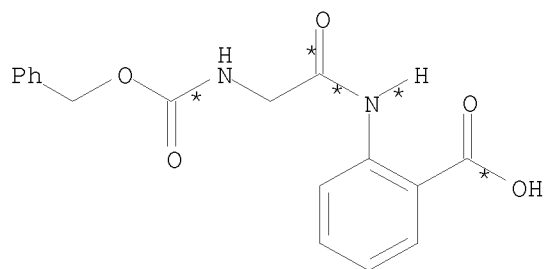
PRO AK 330796-22-0

RX(13) RCT AK 330796-22-0  
RGT AM 1333-74-0 H2  
PRO AL 330796-23-1  
CAT 7440-05-3 Pd  
SOL 64-17-5 EtOH  
CON 2 hours, room temperature

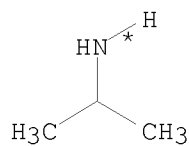
RX(51) OF 105 COMPOSED OF RX(27), RX(26)

RX(51) AG + BQ ==> R

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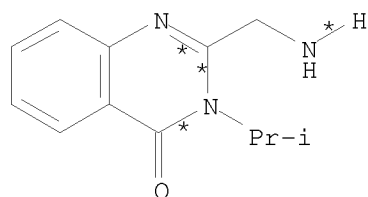


AG



BQ

2  
STEPS  
→



R

YIELD 95%

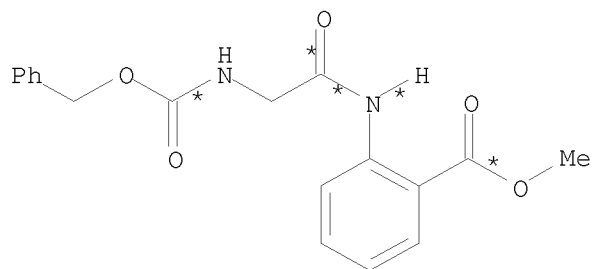
RX(27) RCT AG 55301-19-4, BQ 75-31-0  
RGT AE 530-62-1 Diimidazolyl ketone  
PRO BP 1072784-96-3  
SOL 109-99-9 THF  
CON 20 hours, reflux

RX(26) RCT BP 1072784-96-3  
RGT AM 1333-74-0 H2  
PRO R 1072784-05-4  
CAT 7440-05-3 Pd  
SOL 64-17-5 EtOH  
CON 2 hours, room temperature

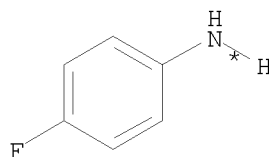
RX(64) OF 105 COMPOSED OF RX(11), RX(12), RX(13)

RX(64) AD + AJ ==> AL

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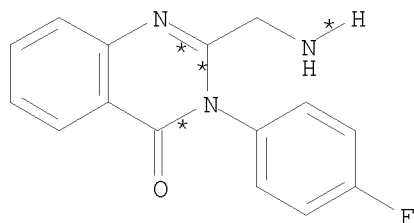


AD



AJ

3  
STEPS  
→



AL  
YIELD 95%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH

SOL 7732-18-5 Water, 123-91-1 Dioxane

CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

CON pH 1

PRO AG 55301-19-4

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone

SOL 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4

SOL 109-99-9 THF

CON 20 hours, room temperature -> 70 deg C

PRO AK 330796-22-0

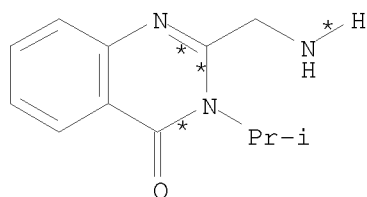
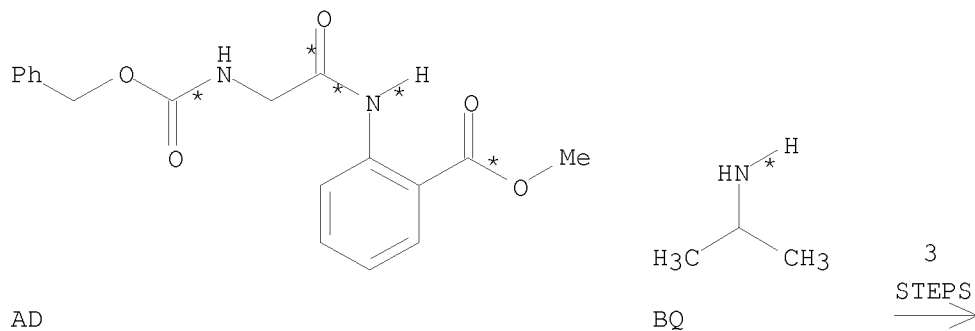
RX(13) RCT AK 330796-22-0

10/ 562,112

RGT AM 1333-74-0 H2  
PRO AL 330796-23-1  
CAT 7440-05-3 Pd  
SOL 64-17-5 EtOH  
CON 2 hours, room temperature

RX(65) OF 105 COMPOSED OF RX(11), RX(27), RX(26)

RX(65) AD + BQ ==> R



R  
YIELD 95%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH  
SOL 7732-18-5 Water, 123-91-1 Dioxane  
CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON pH 1

PRO AG 55301-19-4

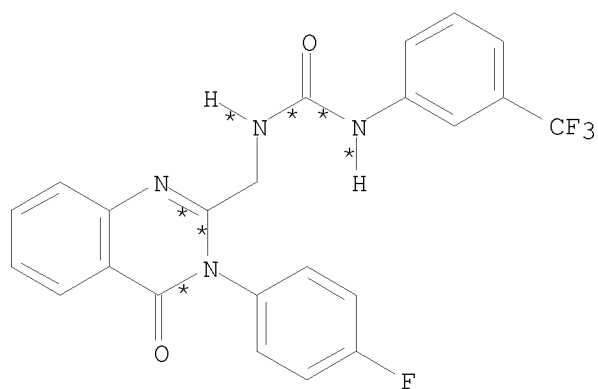
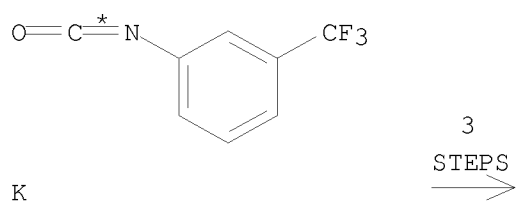
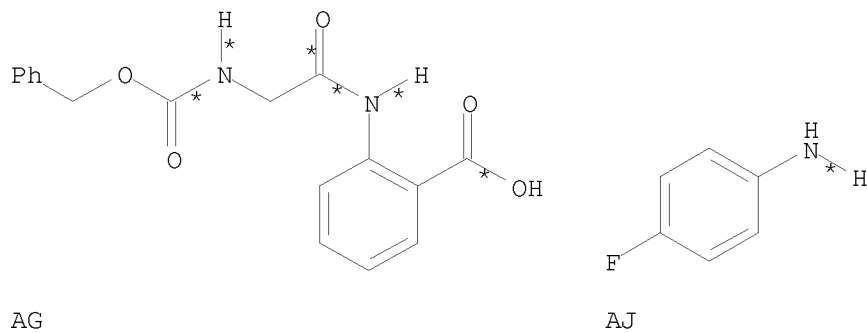
RX(27) RCT AG 55301-19-4, BQ 75-31-0  
RGT AE 530-62-1 Diimidazolyl ketone  
PRO BP 1072784-96-3  
SOL 109-99-9 THF  
CON 20 hours, reflux



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RX(26)      RCT    BP 1072784-96-3  
              RGT    AM 1333-74-0 H2  
              PRO    R 1072784-05-4  
              CAT    7440-05-3 Pd  
              SOL    64-17-5 EtOH  
              CON    2 hours, room temperature

RX(68) OF 105 COMPOSED OF RX(12), RX(13), RX(14)  
RX(68)      AG + AJ + K ==> AO



AO  
YIELD 65%

RX(12)      RCT    AG 55301-19-4

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STAGE(1)

RGT AE 530-62-1 Diimidazoly1 ketone  
SOL 109-99-9 THF  
CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4  
SOL 109-99-9 THF  
CON 20 hours, room temperature -> 70 deg C

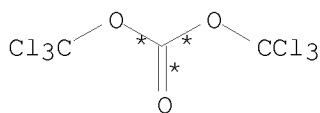
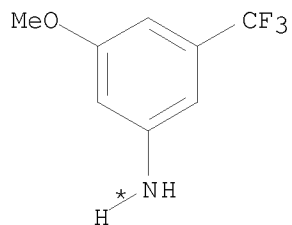
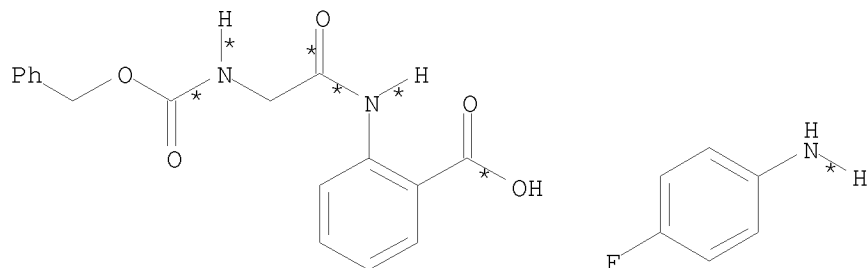
PRO AK 330796-22-0

RX(13) RCT AK 330796-22-0  
RGT AM 1333-74-0 H2  
PRO AL 330796-23-1  
CAT 7440-05-3 Pd  
SOL 64-17-5 EtOH  
CON 2 hours, room temperature

RX(14) RCT K 329-01-1, AL 330796-23-1  
PRO AO 330796-21-9  
SOL 75-09-2 CH2Cl2  
CON 3 hours, room temperature

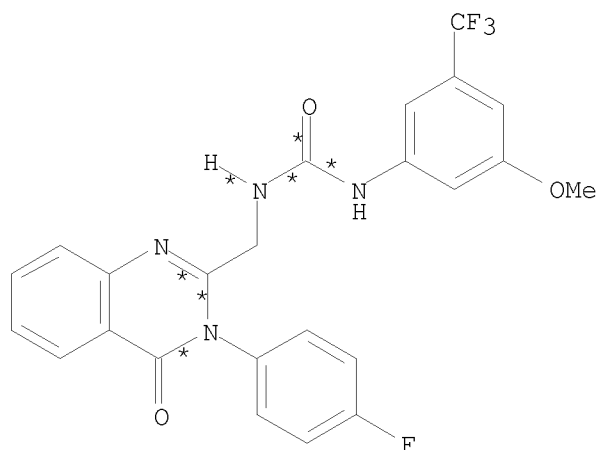
RX(69) OF 105 COMPOSED OF RX(12), RX(13), RX(15)

RX(69) AG + AJ + AQ + AR ==> AS



3  
STEPS  
→

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AS  
YIELD 24%

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone

SOL 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4

SOL 109-99-9 THF

CON 20 hours, room temperature -> 70 deg C

PRO AK 330796-22-0

RX(13) RCT AK 330796-22-0

RGT AM 1333-74-0 H2

PRO AL 330796-23-1

CAT 7440-05-3 Pd

SOL 64-17-5 EtOH

CON 2 hours, room temperature

RX(15) RCT AQ 349-55-3, AR 32315-10-9

STAGE(1)

CAT 7440-44-0 Carbon

SOL 141-78-6 AcOEt

CON 2 hours, room temperature -> 78 deg C

STAGE(2)

RCT AL 330796-23-1

SOL 67-66-3 CHCl3

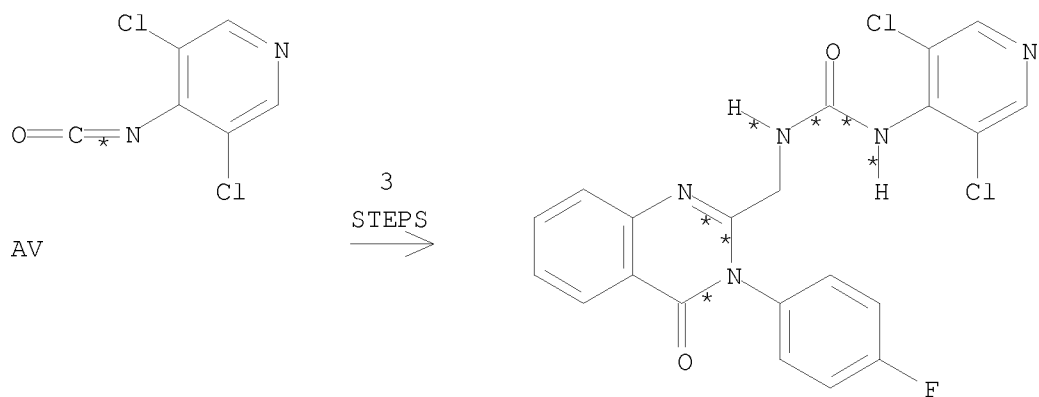
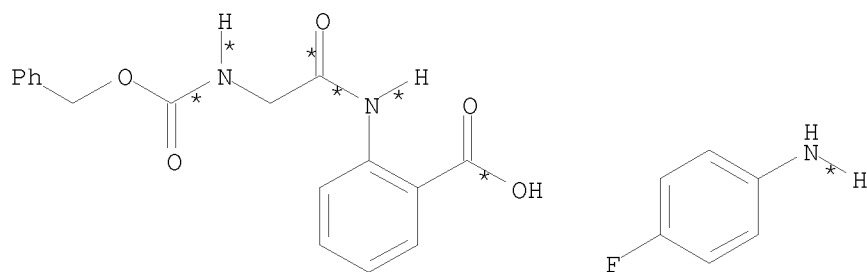
CON 18 hours, room temperature

PRO AS 1016901-87-3

RX(70) OF 105 COMPOSED OF RX(12), RX(13), RX(16)

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RX(70) AG + AJ + AV ==> AW



YIELD 96%

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone

SOL 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4

SOL 109-99-9 THF

CON 20 hours, room temperature -> 70 deg C

PRO AK 330796-22-0

RX(13)

RCT AK 330796-22-0

RGT AM 1333-74-0 H2

PRO AL 330796-23-1

CAT 7440-05-3 Pd

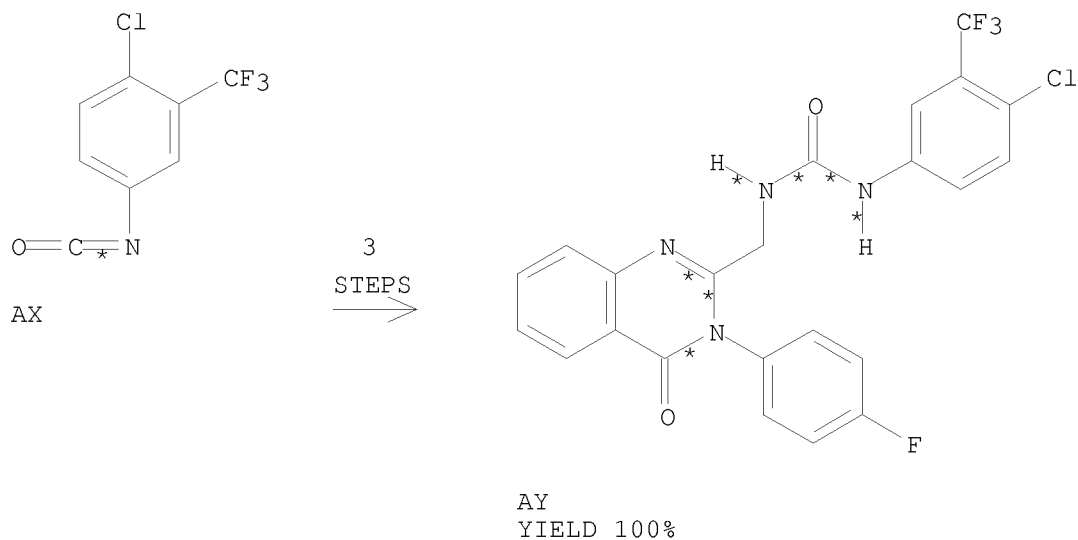
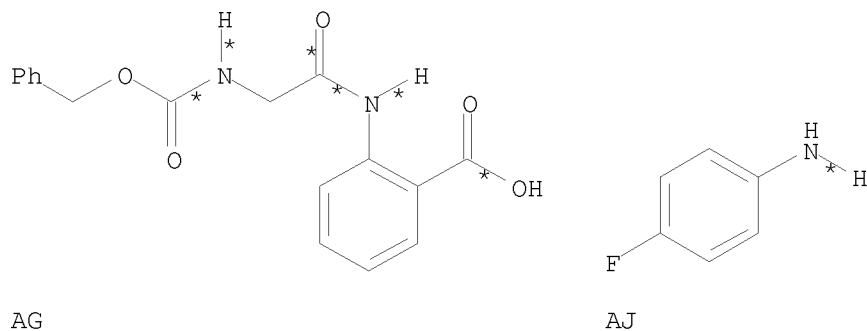
SOL 64-17-5 EtOH

CON 2 hours, room temperature

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RX(16) RCT AL 330796-23-1, AV 481704-32-9  
PRO AW 1016901-88-4  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 3 hours, room temperature

RX(71) OF 105 COMPOSED OF RX(12), RX(13), RX(17)  
RX(71) AG + AJ + AX ==> AY



RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone  
SOL 109-99-9 THF  
CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4  
SOL 109-99-9 THF  
CON 20 hours, room temperature -> 70 deg C

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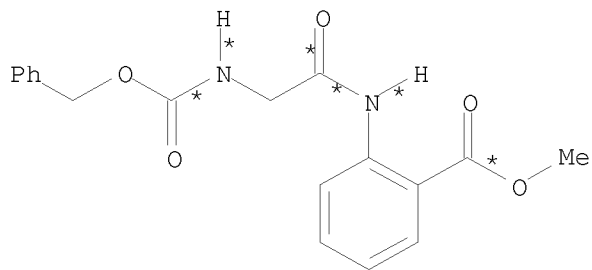
PRO AK 330796-22-0

RX(13) RCT AK 330796-22-0  
RGT AM 1333-74-0 H2  
PRO AL 330796-23-1  
CAT 7440-05-3 Pd  
SOL 64-17-5 EtOH  
CON 2 hours, room temperature

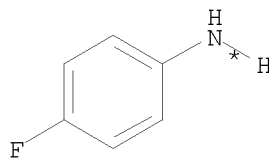
RX(17) RCT AL 330796-23-1, AX 327-78-6  
PRO AY 330796-24-2  
SOL 75-09-2 CH2Cl2  
CON 3 hours, room temperature

RX(72) OF 105 COMPOSED OF RX(11), RX(12), RX(13), RX(14)

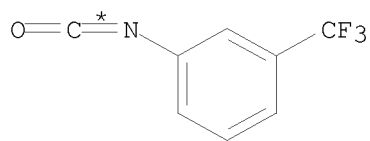
RX(72) AD + AJ + K ==> AO



AD



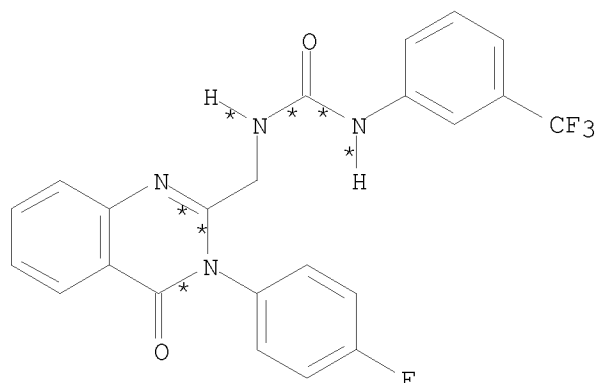
AJ



K

4  
STEPS  
→

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AO  
YIELD 65%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH

SOL 7732-18-5 Water, 123-91-1 Dioxane

CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

CON pH 1

PRO AG 55301-19-4

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone

SOL 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4

SOL 109-99-9 THF

CON 20 hours, room temperature -> 70 deg C

PRO AK 330796-22-0

RX(13) RCT AK 330796-22-0

RGT AM 1333-74-0 H<sub>2</sub>

PRO AL 330796-23-1

CAT 7440-05-3 Pd

SOL 64-17-5 EtOH

CON 2 hours, room temperature

RX(14) RCT K 329-01-1, AL 330796-23-1

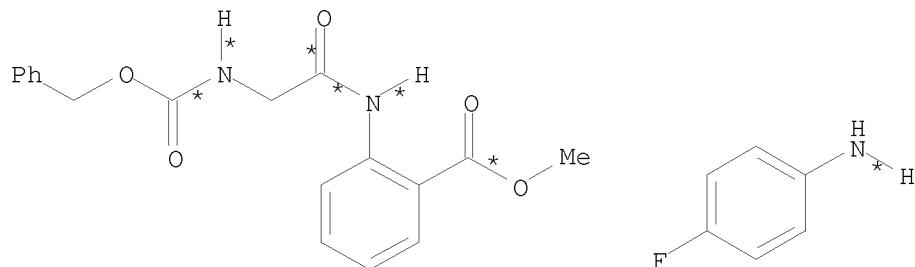
PRO AO 330796-21-9

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON 3 hours, room temperature

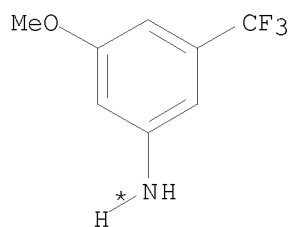
10/ 562,112

RX(73) OF 105 COMPOSED OF RX(11), RX(12), RX(13), RX(15)  
RX(73) AD + AJ + AQ + AR ==> AS

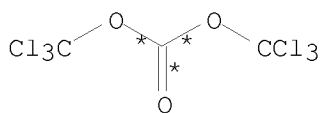


AD

AJ

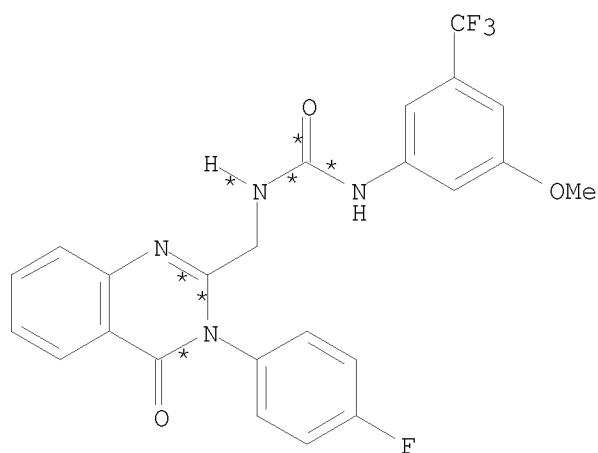


AQ



AR

4  
STEPS  
→



AS  
YIELD 24%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH



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SOL 7732-18-5 Water, 123-91-1 Dioxane  
CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON pH 1

PRO AG 55301-19-4

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone  
SOL 109-99-9 THF  
CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4  
SOL 109-99-9 THF  
CON 20 hours, room temperature -> 70 deg C

PRO AK 330796-22-0

RX(13) RCT AK 330796-22-0  
RGT AM 1333-74-0 H2  
PRO AL 330796-23-1  
CAT 7440-05-3 Pd  
SOL 64-17-5 EtOH  
CON 2 hours, room temperature

RX(15) RCT AQ 349-55-3, AR 32315-10-9

STAGE(1)

CAT 7440-44-0 Carbon  
SOL 141-78-6 AcOEt  
CON 2 hours, room temperature -> 78 deg C

STAGE(2)

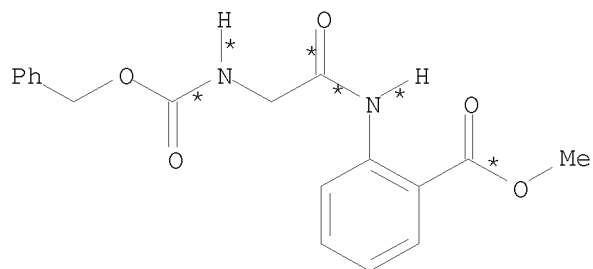
RCT AL 330796-23-1  
SOL 67-66-3 CHCl3  
CON 18 hours, room temperature

PRO AS 1016901-87-3

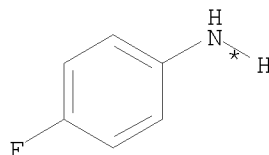
RX(74) OF 105 COMPOSED OF RX(11), RX(12), RX(13), RX(16)

RX(74) AD + AJ + AV ==> AW

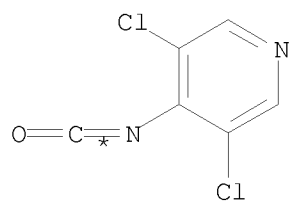
10/ 562,112



AD

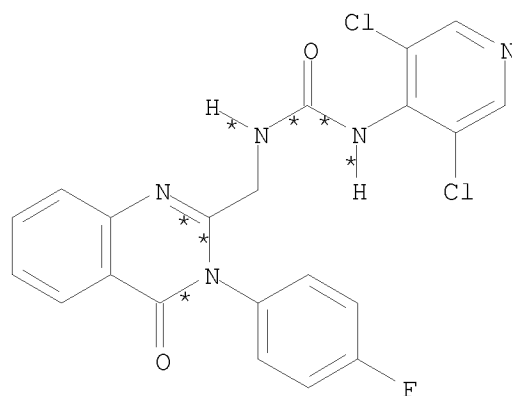


AJ



AV

4  
STEPS  
→



AW  
YIELD 96%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH

SOL 7732-18-5 Water, 123-91-1 Dioxane

CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

CON pH 1

PRO AG 55301-19-4

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone

SOL 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4

10/ 562,112

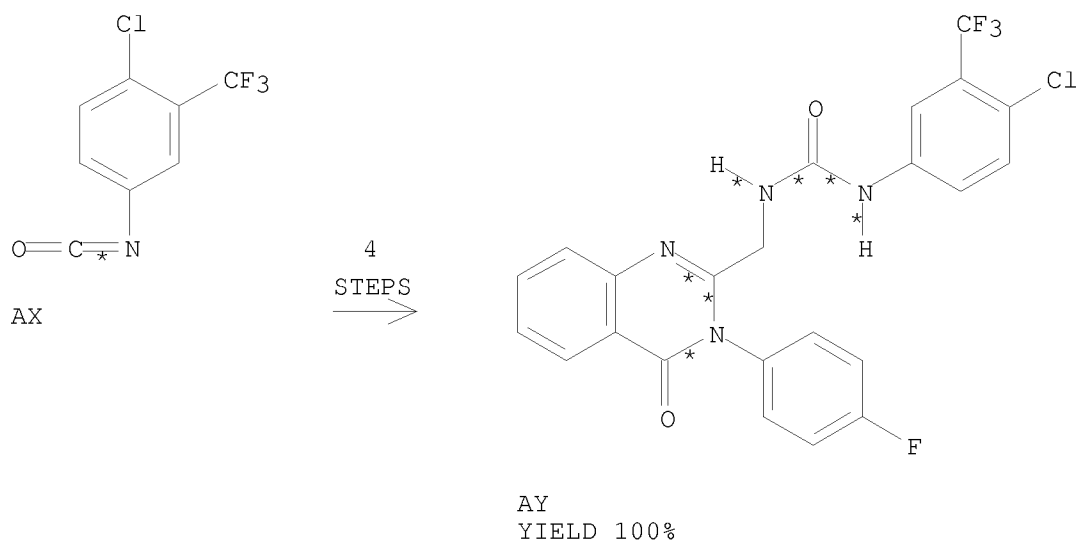
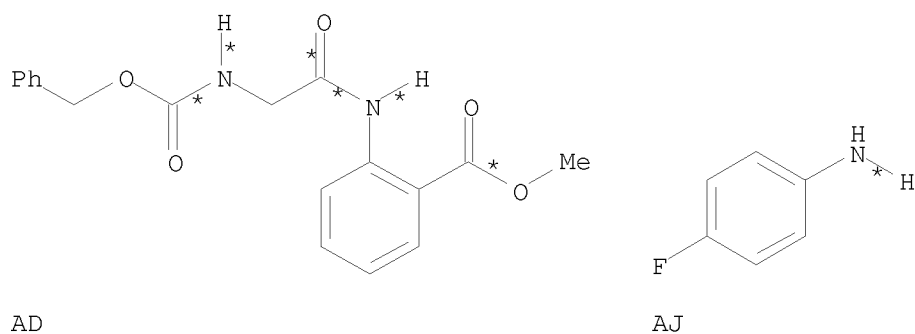
SOL 109-99-9 THF  
CON 20 hours, room temperature -> 70 deg C

PRO AK 330796-22-0

RX(13) RCT AK 330796-22-0  
RGT AM 1333-74-0 H2  
PRO AL 330796-23-1  
CAT 7440-05-3 Pd  
SOL 64-17-5 EtOH  
CON 2 hours, room temperature

RX(16) RCT AL 330796-23-1, AV 481704-32-9  
PRO AW 1016901-88-4  
SOL 75-09-2 CH2Cl2  
CON 3 hours, room temperature

RX(75) OF 105 COMPOSED OF RX(11), RX(12), RX(13), RX(17)  
RX(75) AD + AJ + AX ==> AY



RX(11) RCT AD 133010-41-0

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STAGE(1)

RGT AH 1310-65-2 LiOH  
SOL 7732-18-5 Water, 123-91-1 Dioxane  
CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON pH 1

PRO AG 55301-19-4

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone  
SOL 109-99-9 THF  
CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4  
SOL 109-99-9 THF  
CON 20 hours, room temperature -> 70 deg C

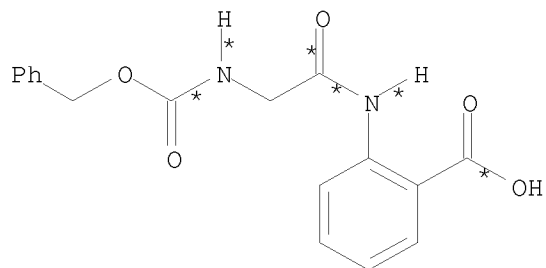
PRO AK 330796-22-0

RX(13) RCT AK 330796-22-0  
RGT AM 1333-74-0 H2  
PRO AL 330796-23-1  
CAT 7440-05-3 Pd  
SOL 64-17-5 EtOH  
CON 2 hours, room temperature

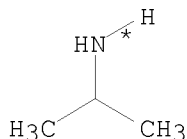
RX(17) RCT AL 330796-23-1, AX 327-78-6  
PRO AY 330796-24-2  
SOL 75-09-2 CH2Cl2  
CON 3 hours, room temperature

RX(85) OF 105 COMPOSED OF RX(27), RX(26), RX(6)

RX(85) AG + BQ + K ==> S

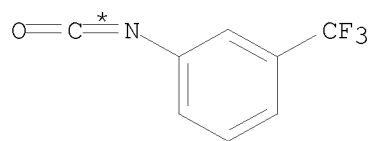


AG



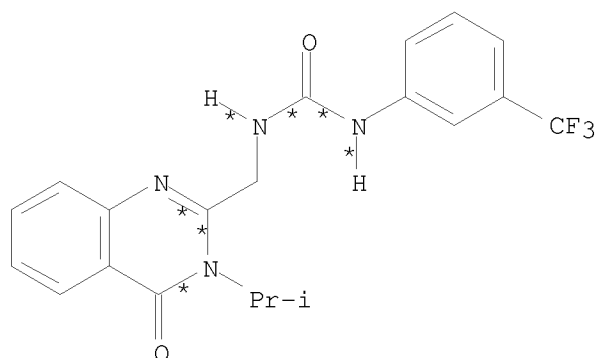
BQ

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K

3  
STEPS  
→



S  
YIELD 11%

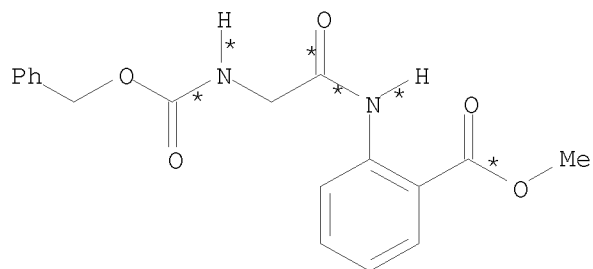
RX(27) RCT AG 55301-19-4, BQ 75-31-0  
RGT AE 530-62-1 Diimidazolyl ketone  
PRO BP 1072784-96-3  
SOL 109-99-9 THF  
CON 20 hours, reflux

RX(26) RCT BP 1072784-96-3  
RGT AM 1333-74-0 H2  
PRO R 1072784-05-4  
CAT 7440-05-3 Pd  
SOL 64-17-5 EtOH  
CON 2 hours, room temperature

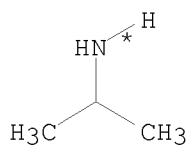
RX(6) RCT K 329-01-1, R 1072784-05-4  
PRO S 1016901-86-2  
SOL 67-66-3 CHCl3  
CON SUBSTAGE(1) 10 minutes, 0 deg C  
SUBSTAGE(2) 1 hour, 0 deg C

RX(86) OF 105 COMPOSED OF RX(11), RX(27), RX(26), RX(6)  
RX(86) AD + BQ + K ==> S

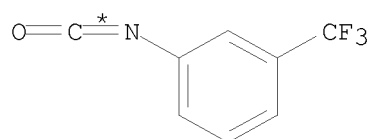
10/ 562,112



AD

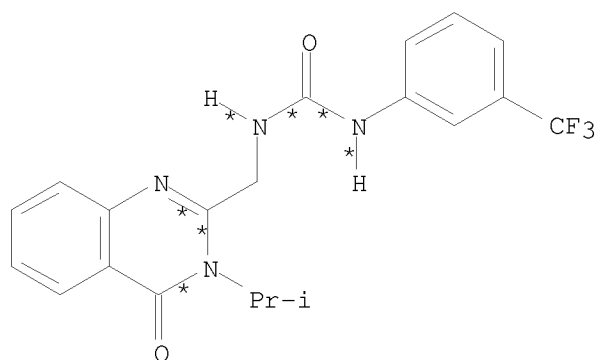


BQ



K

4  
STEPS  
→



S  
YIELD 11%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH

SOL 7732-18-5 Water, 123-91-1 Dioxane

CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

CON pH 1

PRO AG 55301-19-4

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RX(27) RCT AG 55301-19-4, BQ 75-31-0  
RGT AE 530-62-1 Diimidazolyl ketone  
PRO BP 1072784-96-3  
SOL 109-99-9 THF  
CON 20 hours, reflux

RX(26) RCT BP 1072784-96-3  
RGT AM 1333-74-0 H2  
PRO R 1072784-05-4  
CAT 7440-05-3 Pd  
SOL 64-17-5 EtOH  
CON 2 hours, room temperature

RX(6) RCT K 329-01-1, R 1072784-05-4  
PRO S 1016901-86-2  
SOL 67-66-3 CHCl3  
CON SUBSTAGE(1) 10 minutes, 0 deg C  
SUBSTAGE(2) 1 hour, 0 deg C

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 148:379548 CASREACT

TITLE: Bisheterocycles: synthesis of some novel  
1,2,3-triazolyloxadiazole and -4(3H)-quinazolinones  
via azide cycloaddition reaction

AUTHOR(S): Komaraiah, A.; Ramakrishna, K.; Sailu, B.; Reddy, P.  
S. N.

CORPORATE SOURCE: Department of Chemistry, Osmania University,  
Hyderabad, 500007, India

SOURCE: ARKIVOC (Gainesville, FL, United States) (2007), (14),  
110-116

CODEN: AGFUAR

URL: [http://content.arkat-usa.org/ARKIVOC/JOURNAL\\_CONTENT/manuscripts/2007/07-2388MP%20as%20published%20mainmanuscript.pdf](http://content.arkat-usa.org/ARKIVOC/JOURNAL_CONTENT/manuscripts/2007/07-2388MP%20as%20published%20mainmanuscript.pdf)

PUBLISHER: Arkat USA Inc.

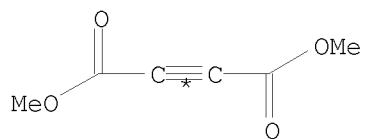
DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

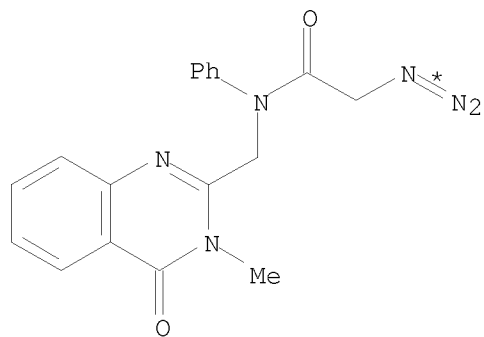
AB 2,5-Bis[2-(4,5-dimethoxycarbonyl)1,2,3-triazol-1-ylacetylaminophenyl]-  
1,3,4-oxadiazole and di-Me 1-(2-[(3-methyl-4-oxo-3,4-dihydro-2-  
quinazolinyl)methyl]anilino)-2-oxoethyl)-1H-1,2,3-triazole-4,5-  
dicarboxylate are prepared by cycloaddn. of di-Me acetylenedicarboxylate to  
2,5-bis(2-azidoacetylaminophenyl)1,3,4-oxadiazole and  
2-(N-aryl-N-azidoacetylaminomethyl)-3-methylquinazolin-4-one, resp.

RX(4) OF 11 H + K ==> L

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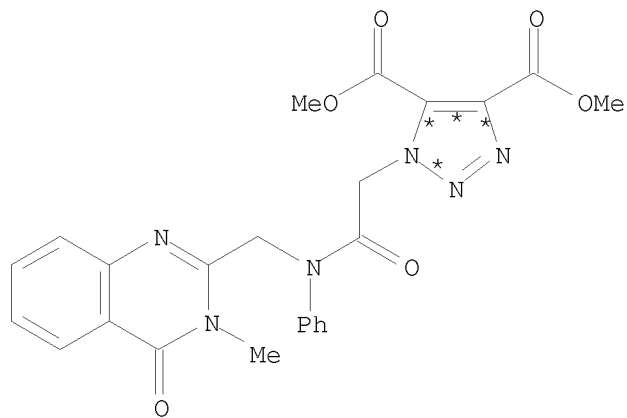


H



K

(4)  $\longrightarrow$



L

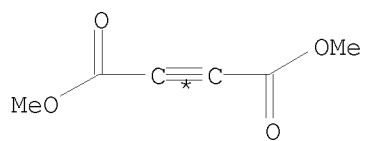
YIELD 74%

RX(4)      RCT   H 762-42-5, K 536697-61-7  
              PRO   L 1014987-15-5  
              SOL   67-64-1 Me<sub>2</sub>CO  
              CON   12 - 14 hours, reflux

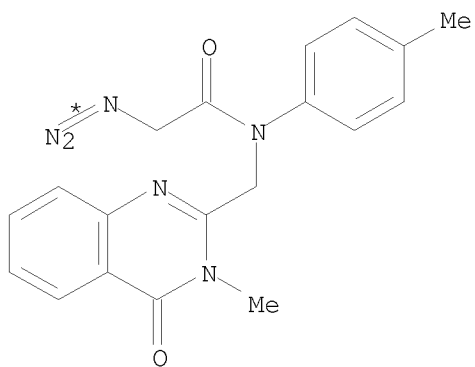
RX(5) OF 11      H + M ==> N



10/ 562,112

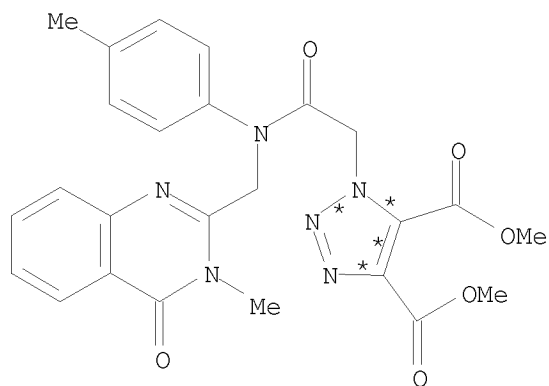


H



M

(5)  $\longrightarrow$



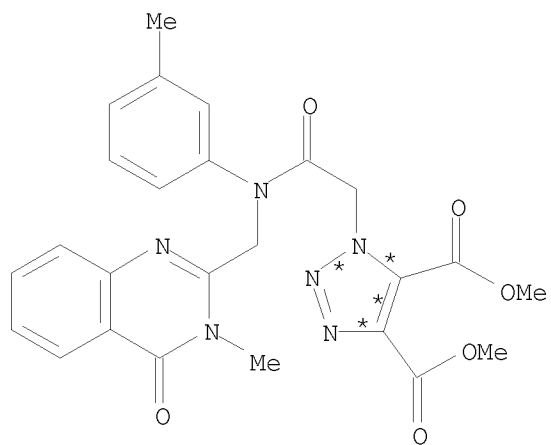
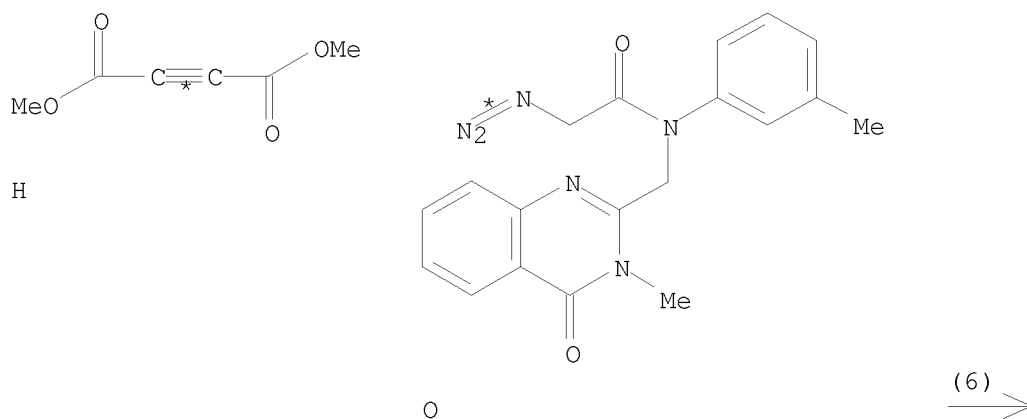
N

YIELD 79%

RX(5) RCT H 762-42-5, M 536697-62-8  
 PRO N 1014987-16-6  
 SOL 67-64-1 Me2CO  
 CON 12 - 14 hours, reflux

RX(6) OF 11 H + O ==> P

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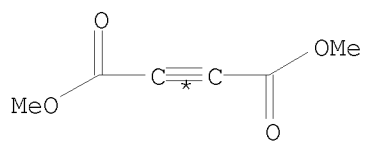


P  
YIELD 77%

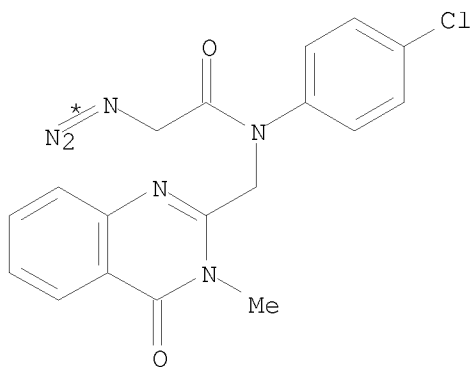
RX(6) RCT H 762-42-5, O 1014987-13-3  
PRO P 1014987-17-7  
SOL 67-64-1 Me<sub>2</sub>CO  
CON 12 - 14 hours, reflux

RX(7) OF 11 H + Q ==> R

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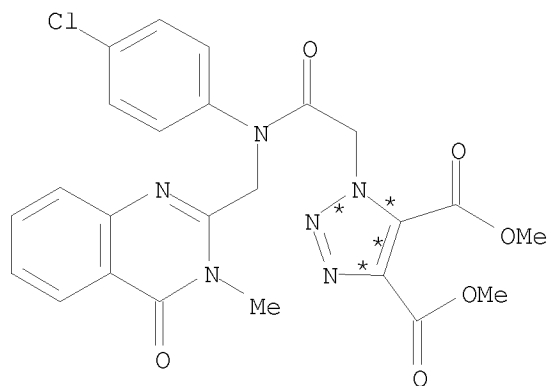


H



Q

(7)  $\longrightarrow$



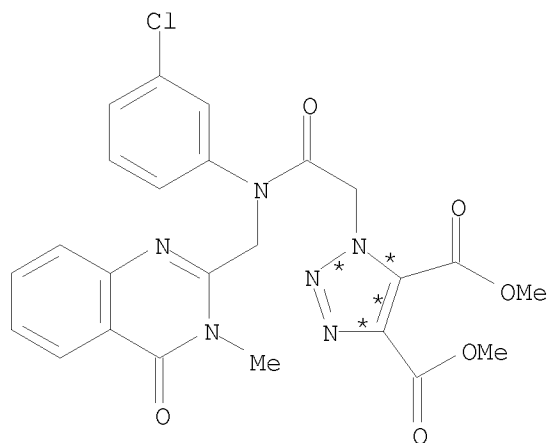
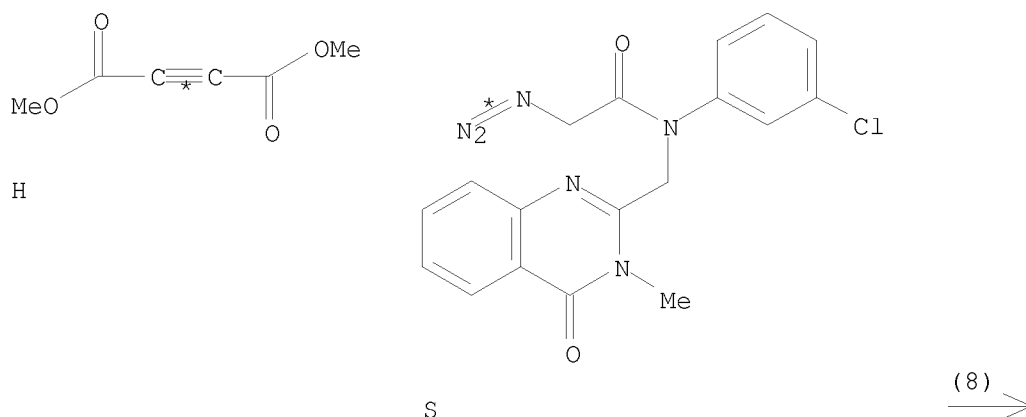
R

YIELD 69%

RX(7) RCT H 762-42-5, Q 536697-64-0  
 PRO R 1014987-18-8  
 SOL 67-64-1 Me2CO  
 CON 12 - 14 hours, reflux

RX(8) OF 11 H + S ==> T

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T  
YIELD 73%

RX(8) RCT H 762-42-5, S 1014987-14-4  
PRO T 1014987-19-9  
SOL 67-64-1 Me2CO  
CON 12 - 14 hours, reflux

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 148:355656 CASREACT  
TITLE: Use of 2-(substituted vinyl)-4(3H)-quinazolinone and -4H-3,1-benzoxazinone in synthesis of heterocycles  
AUTHOR(S): Morsy, J. M.  
CORPORATE SOURCE: Chemistry Department, Faculty of Education, Ain Shams University, Cairo, Egypt  
SOURCE: Bulgarian Chemical Communications (2007), 39(2),

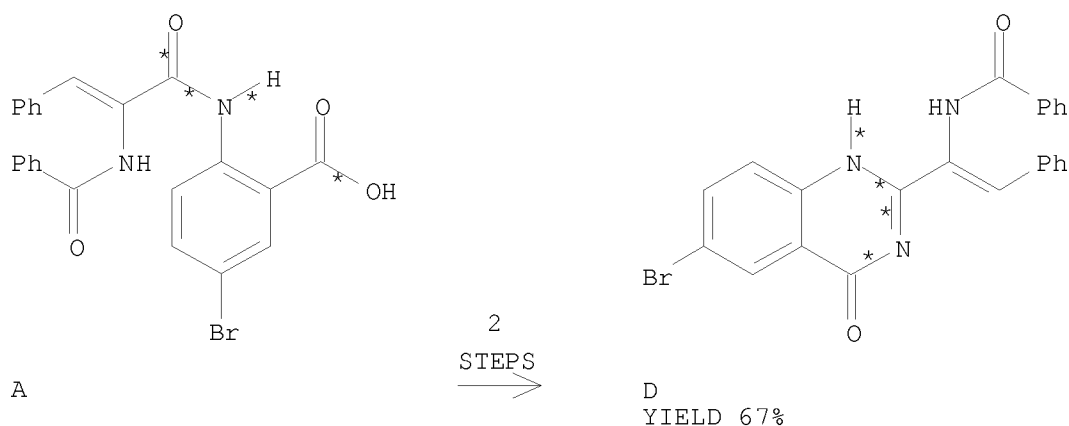
146-151  
 CODEN: BCHCE4; ISSN: 0324-1130  
 Bulgarian Academy of Sciences  
 Journal  
 English

PUBLISHER:  
 DOCUMENT TYPE:  
 LANGUAGE:  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB 4H-3,1-Benzoxazinone I was transformed into 4(3H)-quinazolinones II (R = H, NH<sub>2</sub>), which were converted to tetrazole III and thiazole IV in two-step processes. Tetrazole derivative V was also obtained from the starting benzoxazinone in a one-pot facile synthesis.

RX(18) OF 45 COMPOSED OF RX(1), RX(2)  
 RX(18) A ==> D

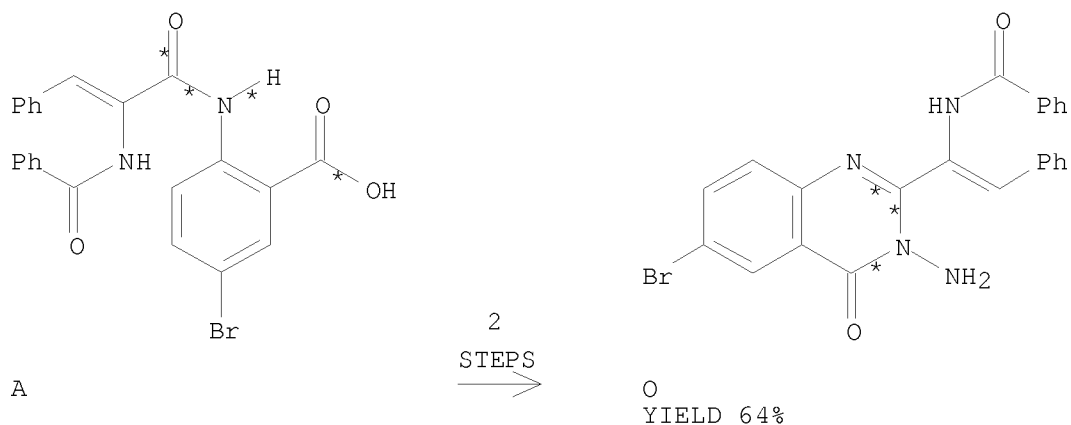


RX(1) RCT A 1012086-13-3  
 RGT C 108-24-7 Ac2O  
 PRO B 1012085-96-9  
 SOL 108-24-7 Ac2O  
 CON 1 hour, 100 deg C

RX(2) RCT B 1012085-96-9  
 RGT E 75-12-7 Formamide  
 PRO D 1012085-97-0  
 SOL 75-12-7 Formamide  
 CON 3 hours, reflux  
 NTE alternative reaction conditions shown

RX(19) OF 45 COMPOSED OF RX(1), RX(6)  
 RX(19) A ==> O

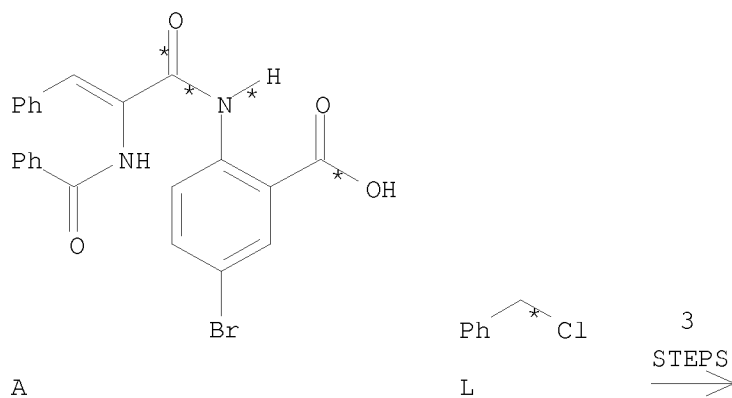
10/ 562,112



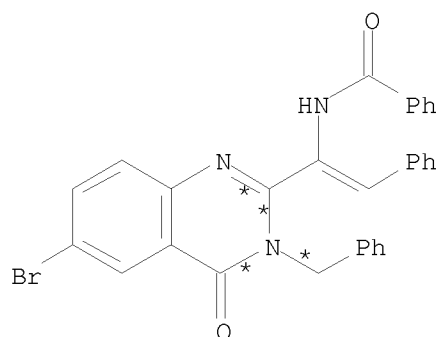
RX(1)      RCT    A 1012086-13-3  
               RGT    C 108-24-7 Ac2O  
               PRO    B 1012085-96-9  
               SOL    108-24-7 Ac2O  
               CON    1 hour, 100 deg C

RX(6)      RCT    B 1012085-96-9  
               RGT    P 7803-57-8 N2H4-H2O  
               PRO    O 1012086-01-9  
               SOL    64-17-5 EtOH  
               CON    3 hours, reflux

RX(35) OF 45 COMPOSED OF RX(1), RX(2), RX(5)  
 RX(35)      A + L ==> M



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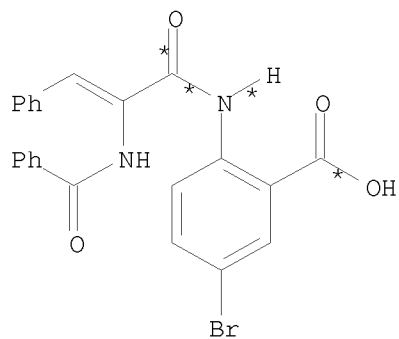
M  
YIELD 62%

RX(1) RCT A 1012086-13-3  
RGT C 108-24-7 Ac2O  
PRO B 1012085-96-9  
SOL 108-24-7 Ac2O  
CON 1 hour, 100 deg C

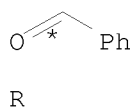
RX(2) RCT B 1012085-96-9  
RGT E 75-12-7 Formamide  
PRO D 1012085-97-0  
SOL 75-12-7 Formamide  
CON 3 hours, reflux  
NTE alternative reaction conditions shown

RX(5) RCT D 1012085-97-0, L 100-44-7  
RGT N 110-86-1 Pyridine  
PRO M 1012086-00-8  
SOL 110-86-1 Pyridine  
CON 3 hours, reflux

RX(36) OF 45 COMPOSED OF RX(1), RX(6), RX(7)  
RX(36) A + R ==> S

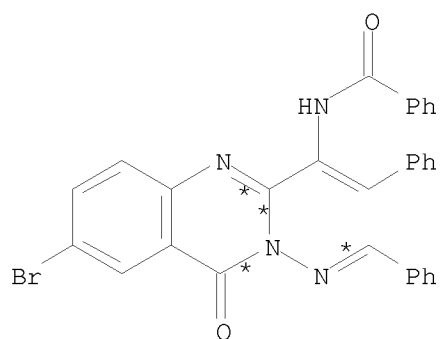


A



3  
STEPS  
→

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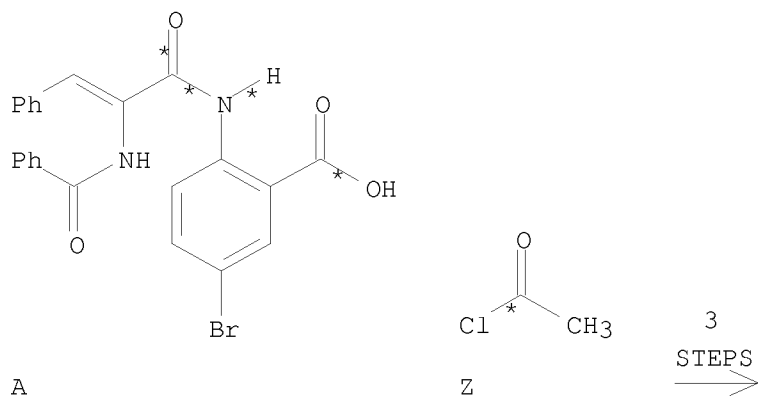
S  
YIELD 55%

RX(1)      RCT    A 1012086-13-3  
             RGT    C 108-24-7 Ac2O  
             PRO    B 1012085-96-9  
             SOL    108-24-7 Ac2O  
             CON    1 hour, 100 deg C

RX(6)      RCT    B 1012085-96-9  
             RGT    P 7803-57-8 N2H4-H2O  
             PRO    O 1012086-01-9  
             SOL    64-17-5 EtOH  
             CON    3 hours, reflux

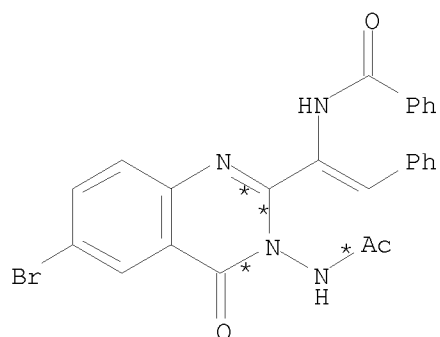
RX(7)      RCT    O 1012086-01-9, R 100-52-7  
             PRO    S 1012086-02-0  
             CAT    110-89-4 Piperidine  
             SOL    64-17-5 EtOH  
             CON    4 hours, reflux

RX(37) OF 45 COMPOSED OF RX(1), RX(6), RX(10)  
RX(37)      A + Z ==> AA





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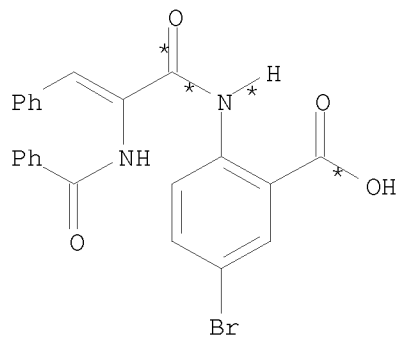
AA  
YIELD 72%

RX(1) RCT A 1012086-13-3  
RGT C 108-24-7 Ac2O  
PRO B 1012085-96-9  
SOL 108-24-7 Ac2O  
CON 1 hour, 100 deg C

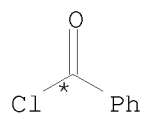
RX(6) RCT B 1012085-96-9  
RGT P 7803-57-8 N2H4-H2O  
PRO O 1012086-01-9  
SOL 64-17-5 EtOH  
CON 3 hours, reflux

RX(10) RCT O 1012086-01-9, Z 75-36-5  
RGT N 110-86-1 Pyridine  
PRO AA 1012086-05-3  
SOL 110-86-1 Pyridine  
CON 3 hours, reflux

RX(38) OF 45 COMPOSED OF RX(1), RX(6), RX(11)  
RX(38) A + AB ==> AC



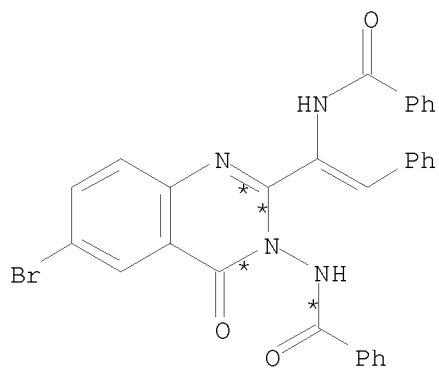
A



AB

3  
STEPS  
=>

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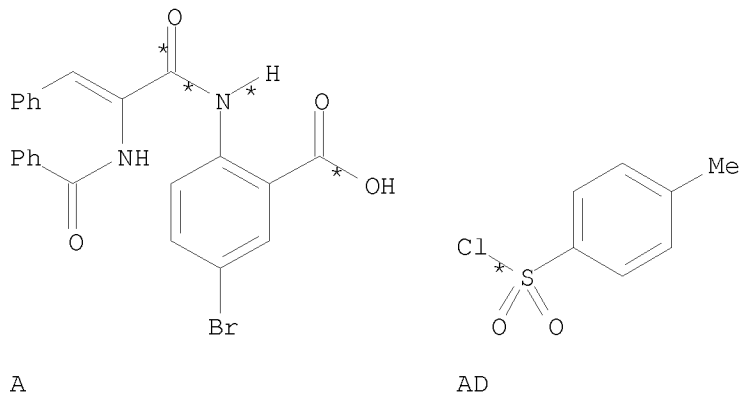
AC  
YIELD 57%

RX (1)            RCT    A 1012086-13-3  
                     RGT    C 108-24-7   Ac2O  
                     PRO    B 1012085-96-9  
                     SOL    108-24-7   Ac2O  
                     CON    1 hour, 100 deg C

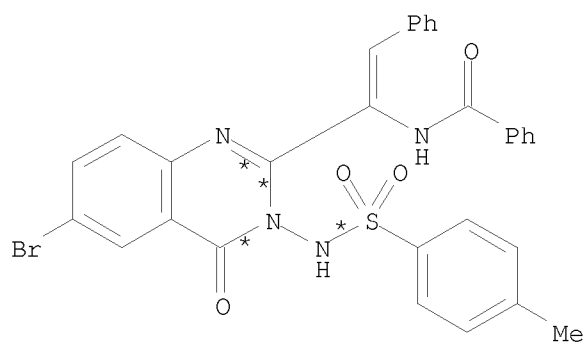
RX (6)	RCT	B	1012085-96-9
	RGT	P	7803-57-8 N2H4-H2O
	PRO	O	1012086-01-9
	SOL		64-17-5 EtOH
	CON		3 hours, reflux

RX(11)	RCT	O 1012086-01-9, AB 98-88-4
	RGT	N 110-86-1 Pyridine
	PRO	AC 1012086-06-4
	SOL	110-86-1 Pyridine
	CON	3 hours, reflux

RX(39) OF 45 COMPOSED OF RX(1), RX(6), RX(12)  
 RX(39) A + AD ==> AE



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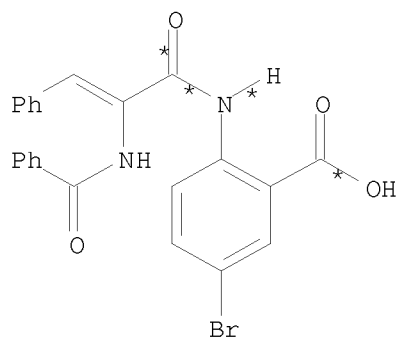
AE  
YIELD 50%

RX(1) RCT A 1012086-13-3  
RGT C 108-24-7 Ac2O  
PRO B 1012085-96-9  
SOL 108-24-7 Ac2O  
CON 1 hour, 100 deg C

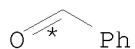
RX(6) RCT B 1012085-96-9  
RGT P 7803-57-8 N2H4-H2O  
PRO O 1012086-01-9  
SOL 64-17-5 EtOH  
CON 3 hours, reflux

RX(12) RCT O 1012086-01-9, AD 98-59-9  
RGT N 110-86-1 Pyridine  
PRO AE 1012086-07-5  
SOL 110-86-1 Pyridine  
CON 4 hours, reflux

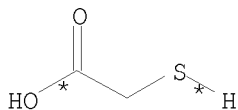
RX(44) OF 45 COMPOSED OF RX(1), RX(6), RX(7), RX(8)  
RX(44) A + R + U ==> V



A



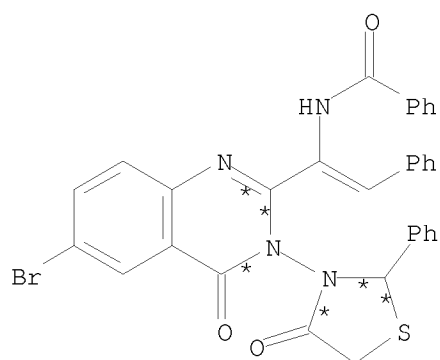
R



U

4  
STEPS  
→

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V

YIELD 67%

RX(1) RCT A 1012086-13-3  
RGT C 108-24-7 Ac2O  
PRO B 1012085-96-9  
SOL 108-24-7 Ac2O  
CON 1 hour, 100 deg C

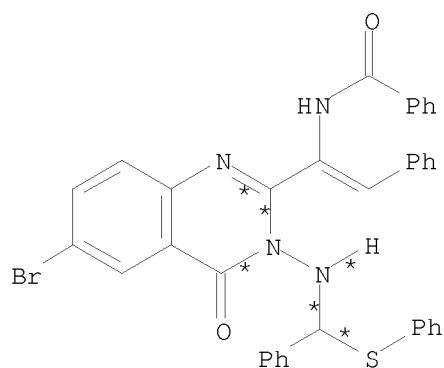
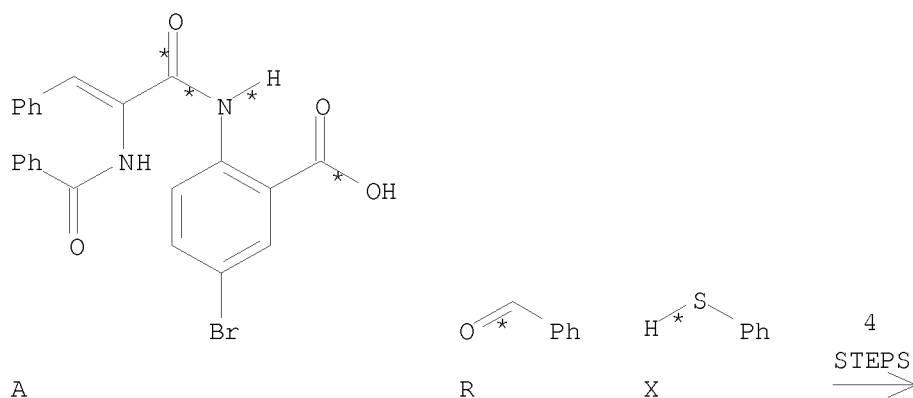
RX(6) RCT B 1012085-96-9  
RGT P 7803-57-8 N2H4-H2O  
PRO O 1012086-01-9  
SOL 64-17-5 EtOH  
CON 3 hours, reflux

RX(7) RCT O 1012086-01-9, R 100-52-7  
PRO S 1012086-02-0  
CAT 110-89-4 Piperidine  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(8) RCT S 1012086-02-0, U 68-11-1  
PRO V 1012086-03-1  
CAT 110-89-4 Piperidine  
SOL 71-43-2 Benzene  
CON 3 hours, reflux

RX(45) OF 45 COMPOSED OF RX(1), RX(6), RX(7), RX(9)  
RX(45) A + R + X ==> Y

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Y  
YIELD 57%

RX(1)	RCT	A 1012086-13-3
	RGT	C 108-24-7 Ac2O
	PRO	B 1012085-96-9
	SOL	108-24-7 Ac2O
	CON	1 hour, 100 deg C
RX(6)	RCT	B 1012085-96-9
	RGT	P 7803-57-8 N2H4-H2O
	PRO	O 1012086-01-9
	SOL	64-17-5 EtOH
	CON	3 hours, reflux
RX(7)	RCT	O 1012086-01-9, R 100-52-7
	PRO	S 1012086-02-0
	CAT	110-89-4 Piperidine
	SOL	64-17-5 EtOH
	CON	4 hours, reflux
RX(9)	RCT	S 1012086-02-0, X 108-98-5
	PRO	Y 1012086-04-2
	CAT	110-89-4 Piperidine
	SOL	71-43-2 Benzene

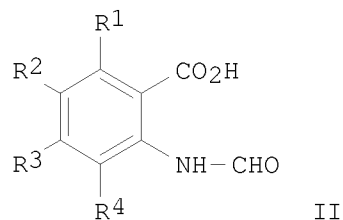
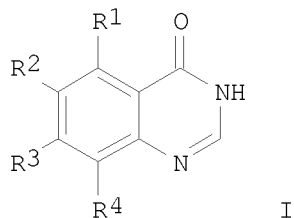
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CON 2 hours, reflux

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 147:502385 CASREACT  
TITLE: Preparation of quinazolin-4-ones from  
N-formylanthranilic acids  
INVENTOR(S): Tanaka, Kazuo; Sato, Yoshifumi; Yoshimura, Takashi  
PATENT ASSIGNEE(S): Mitsubishi Gas Chemical Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 9pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

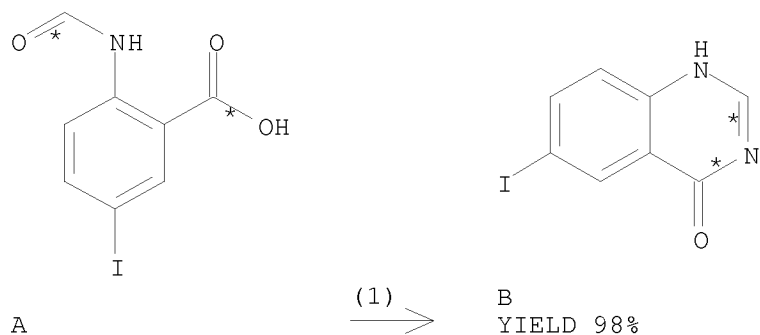
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 2007290974	A	20071108	JP 2006-117729	20060421
PRIORITY APPLN. INFO.:			JP 2006-117729	20060421
OTHER SOURCE(S):	MARPAT 147:502385			
GI				



AB Quinazolin-4-ones I (R1-R4 = H, halo, NO2, C1-6 alkyl, alkoxy) are prepared by treatment of N-formylanthranilic acids II (R1-R4 = same as above) with HCONH2 and ammonia in the presence of AcOH and/or AcNH4 as catalyst. Thus, formylation of 5-iodoanthranilic acid with HCONH2 at 100° for 2 h gave 96.7% N-formyl-5-iodoanthranilic acid with 97.1% purity, which was autoclaved with HCONH2, AcNH4, and ammonia/MeOH at 150° for 2 h to afford 98.0% 6-iodoquinazolin-4-one.

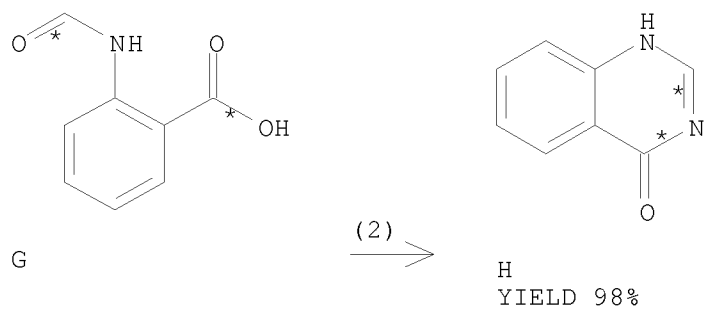
RX(1) OF 4 A ==> B

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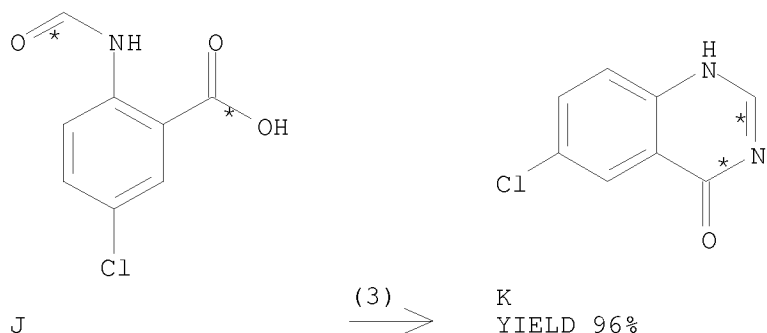
RX(1) RCT A 955998-77-3  
RGT C 75-12-7 Formamide, D 7664-41-7 NH<sub>3</sub>, E 631-61-8 NH<sub>4</sub>OAc  
PRO B 16064-08-7  
SOL 7732-18-5 Water  
CON 2 hours, 150 deg C

RX(2) OF 4 G ==> H



RX(2) RCT G 3342-77-6  
RGT C 75-12-7 Formamide, D 7664-41-7 NH<sub>3</sub>, I 64-19-7 AcOH  
PRO H 491-36-1  
SOL 7732-18-5 Water  
CON 2 hours, 150 deg C

RX(3) OF 4 J ==> K



RX(3) RCT J 26208-56-0  
 RGT C 75-12-7 Formamide, D 7664-41-7 NH3, I 64-19-7 AcOH  
 PRO K 16064-14-5  
 SOL 7732-18-5 Water  
 CON 2 hours, 150 deg C

L3 ANSWER 9 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 147:486453 CASREACT  
 TITLE: Quinazolin-4-one derivatives as B-Raf inhibitors,  
 process for their preparation and pharmaceutical  
 compositions containing them for treating cancer  
 INVENTOR(S): Aquila, Brian; Lyne, Paul; Pontz, Timothy  
 PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca Uk Limited  
 SOURCE: PCT Int. Appl., 52pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

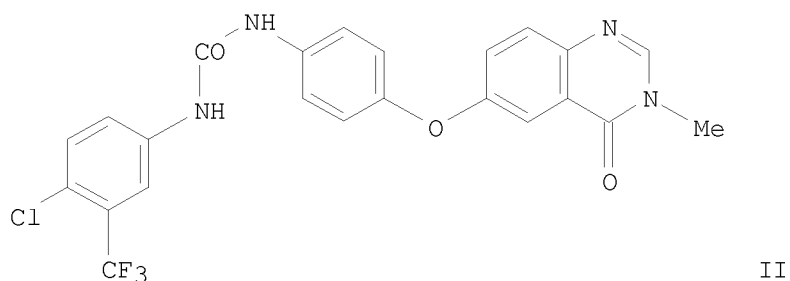
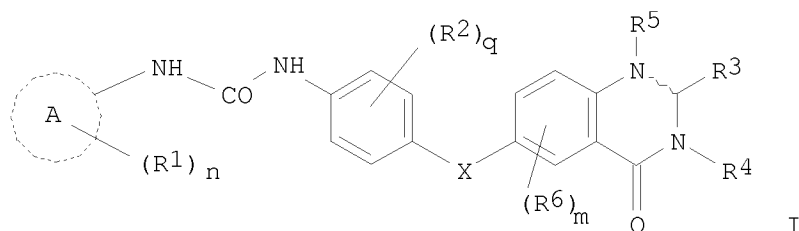
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007119055	A1	20071025	WO 2007-GB1389	20070417
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 2010504	A1	20090107	EP 2007-732431	20070417
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, RS				

PRIORITY APPLN. INFO.:

US 2006-745038P 20060418



OTHER SOURCE(S): MARPAT 147:486453  
GI



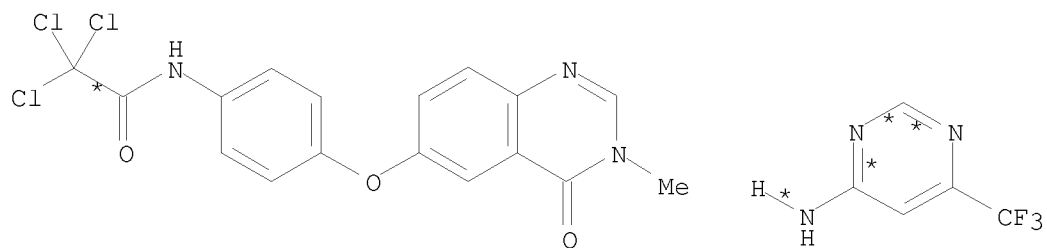
AB The invention relates to chemical compds. of the formula I (wherein Ring A is carbocyclyl or heterocyclyl; R1 is a substituent on C and is halo, nitro, etc.; n is 0-4; R2 is halo, nitro, cyano, OH, etc.; q is 0-2; X is NR16 or O; R3 and R6 are H, halo, nitro, cyano, etc.; R4, R5 and R16 are H, C1-6alkyl, C1-6alkanoyl, etc.; m is 3 wherein the value of R6 may be the same or different) or pharmaceutically acceptable salts thereof, which possess B-Raf inhibitory activity and are accordingly useful for their anti-cancer activity and thus in methods of treatment of the human or animal body. The invention also relates to processes for the manufacture of said chemical compds., to pharmaceutical compns. containing them and to their use

in the manufacture of medicaments of use in the production of an anti-cancer effect

in a warm-blooded animal such as man. Example compound II was prepared by reacting 1-chloro-4-isocyanato-2-(trifluoromethyl)benzene and 6-(4-aminophenoxy)-3-methylquinazolin-4(3H)-one. In the B-Raf in vitro AlphaScreen assay, II had an IC50 of 0.287  $\mu$ M.

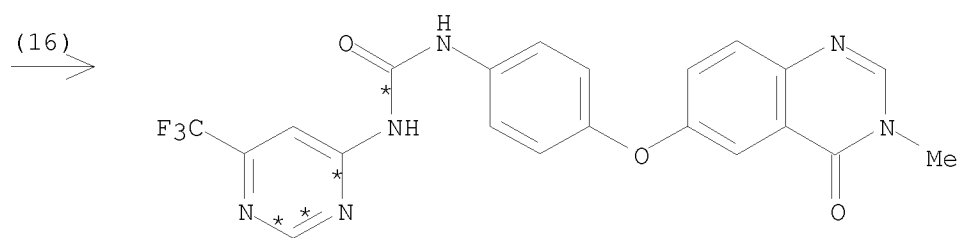
RX(16) OF 215 ...AL + AM ==> AN

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AL

AM



AN  
YIELD 35%

RX(16) RCT AL 953414-07-8, AM 672-41-3

STAGE(1)

RGT AO 1310-73-2 NaOH

SOL 67-68-5 DMSO

CON SUBSTAGE(1) 80 deg C

SUBSTAGE(2) 80 deg C -> 25 deg C

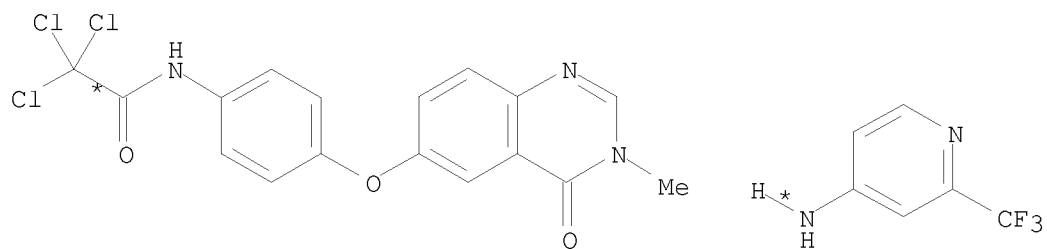
STAGE(2)

RGT AP 7732-18-5 Water

CON 25 deg C

PRO AN 953414-03-4

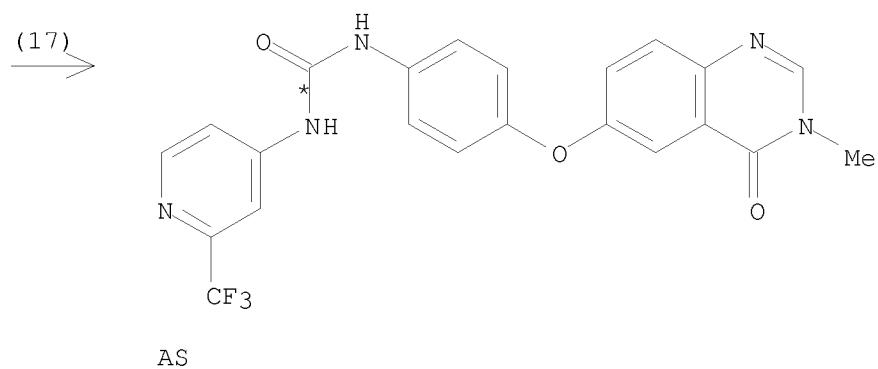
RX(17) OF 215 ...AL + AR ==> AS



AL

AR

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RX(17) RCT AL 953414-07-8, AR 147149-98-2

STAGE(1)

RGT AO 1310-73-2 NaOH

SOL 67-68-5 DMSO

CON SUBSTAGE(1) 80 deg C

SUBSTAGE(2) 80 deg C -> 25 deg C

STAGE(2)

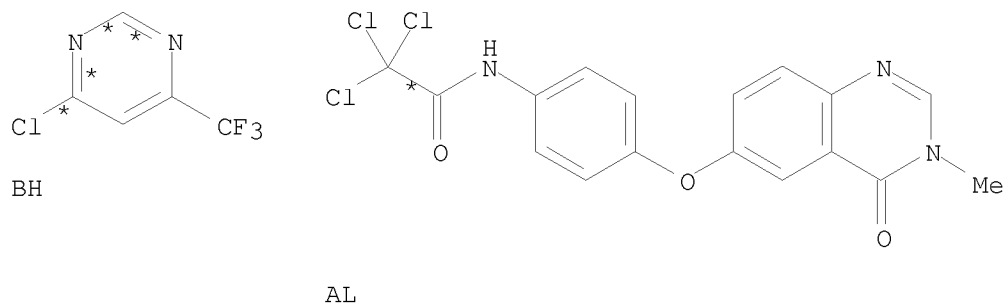
RGT AP 7732-18-5 Water

CON 25 deg C

PRO AS 953414-04-5

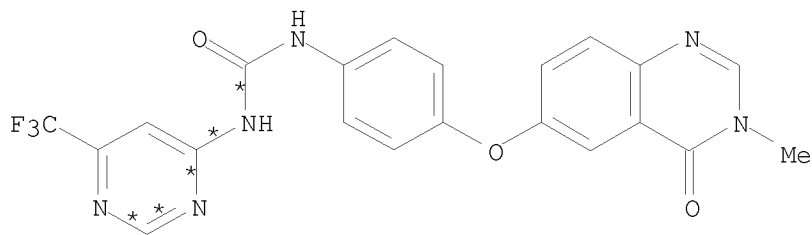
RX(66) OF 215 COMPOSED OF RX(23), RX(16)

RX(66) BH + AL ==> AN



2  
STEPS  


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AN  
YIELD 35%

RX(23)      RCT   BH 37552-81-1  
              RGT   BI 7664-41-7 NH3  
              PRO   AM 672-41-3  
              SOL   67-56-1 MeOH  
              CON   12 hours, 25 deg C  
              NTE   overall yield is 29% over two steps

RX(16) RCT AL 953414-07-8, AM 672-41-3

STAGE (1)

RGT AO 1310-73-2 NaOH

SOL 67-68-5 DMSO

CON SUBSTAGE (1) 80 deg C

SUBSTAGE (2) 80 deg C -> 25 deg C

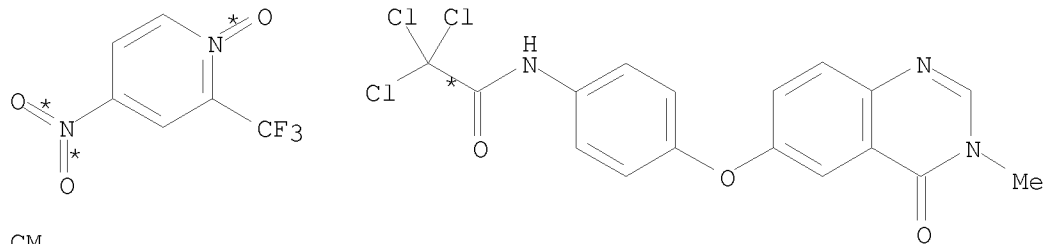
STAGE (2)

RGT AP 7732-18-5 Water

CON 25 deg C

PRO AN 953414-03-4

RX(90) OF 215 COMPOSED OF RX(43), RX(17)

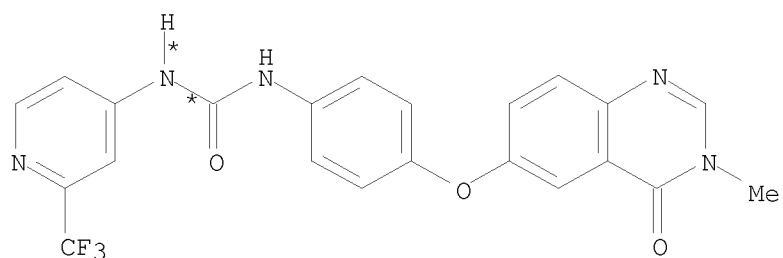
$$\text{RX}(90) \quad \text{CM} \quad + \quad \text{AL} \quad \Longrightarrow \quad \text{AS}$$


CM

AL

2  
STEPS  
→

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AS

RX(43)     RCT    CM 147149-97-1  
             RGT    AU 1333-74-0 H2  
             PRO    AR 147149-98-2  
             CAT    7440-05-3 Pd  
             SOL    67-56-1 MeOH  
             CON    12 hours, room temperature  
             NTE    overall yield is 9% over two steps

RX(17)     RCT    AL 953414-07-8, AR 147149-98-2

STAGE(1)

             RGT    AO 1310-73-2 NaOH  
             SOL    67-68-5 DMSO  
             CON    SUBSTAGE(1) 80 deg C  
                     SUBSTAGE(2) 80 deg C -> 25 deg C

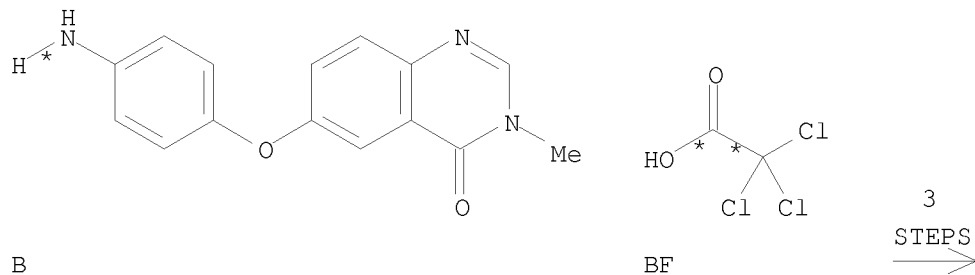
STAGE(2)

             RGT    AP 7732-18-5 Water  
             CON    25 deg C

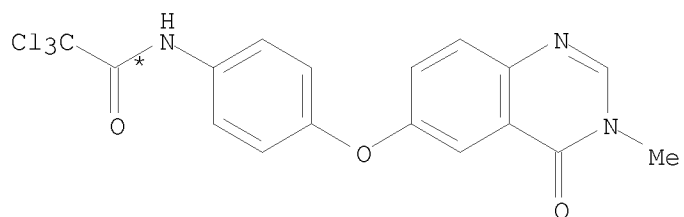
PRO    AS 953414-04-5

RX(115) OF 215 COMPOSED OF REACTION SEQUENCE RX(22), RX(16)  
             AND REACTION SEQUENCE RX(50), RX(23), RX(16)

...B + BF ==> AL...  
...DE + AL ==> AN

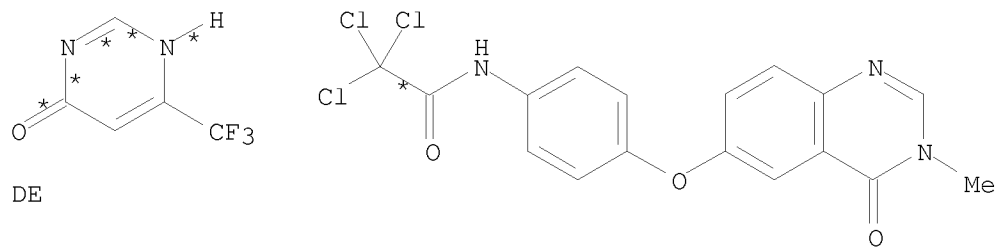


10/ 562,112



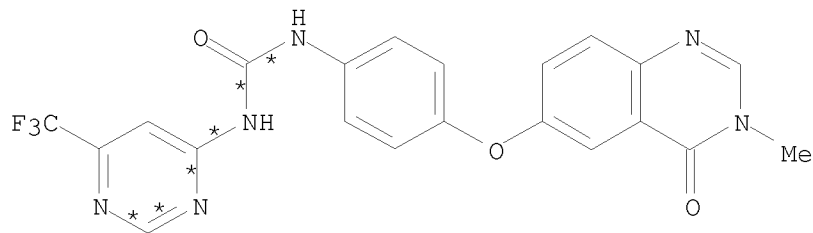
AL

START NEXT REACTION SEQUENCE



AL

3  
STEPS  
→



AN  
YIELD 35%

RX(22) RCT B 953414-05-6, BF 76-03-9

STAGE(1)

RGT BG 7719-12-2 PC13  
CON reflux

STAGE(2)

RGT AP 7732-18-5 Water  
CON cooled

PRO AL 953414-07-8

RX(50)

RCT DE 1546-78-7  
RGT DF 824-72-6 PhP(O)Cl2  
PRO BH 37552-81-1  
CON SUBSTAGE(1) 30 minutes, 130 deg C  
SUBSTAGE(2) 130 deg C -> 25 deg C

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RX(23)     RCT   BH 37552-81-1  
           RGT   BI 7664-41-7 NH3  
           PRO   AM 672-41-3  
           SOL   67-56-1 MeOH  
           CON   12 hours, 25 deg C  
           NTE   overall yield is 29% over two steps

RX(16)     RCT   AL 953414-07-8, AM 672-41-3

           STAGE(1)

             RGT   AO 1310-73-2 NaOH  
             SOL   67-68-5 DMSO  
             CON   SUBSTAGE(1) 80 deg C  
                     SUBSTAGE(2) 80 deg C -> 25 deg C

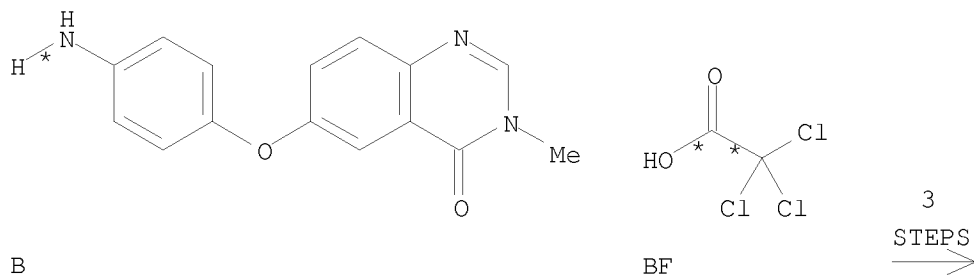
           STAGE(2)

             RGT   AP 7732-18-5 Water  
             CON   25 deg C

           PRO   AN 953414-03-4

RX(168) OF 215 COMPOSED OF REACTION SEQUENCE RX(22), RX(17)  
                                 AND REACTION SEQUENCE RX(44), RX(43), RX(17)

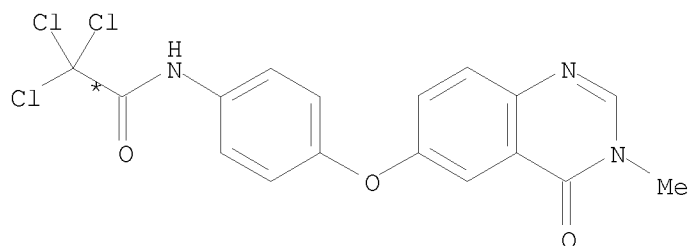
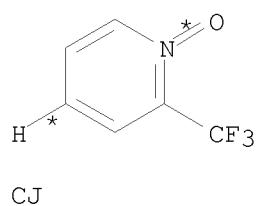
...B   +   BF   ==>   AL...  
...CJ   +   AL   ==>   AS



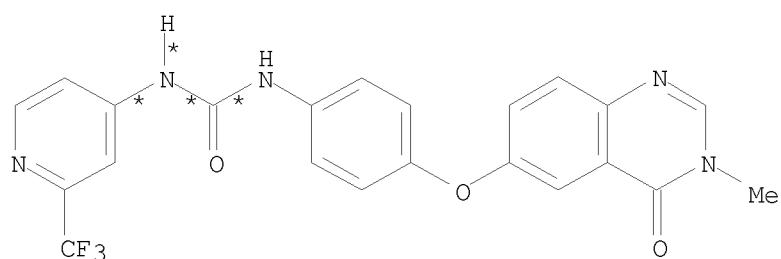
AL

START NEXT REACTION SEQUENCE

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3  
STEPS  
→



RX(22) RCT B 953414-05-6, BF 76-03-9

STAGE(1)

RGT BG 7719-12-2 PC13  
CON reflux

STAGE(2)

RGT AP 7732-18-5 Water  
CON cooled

PRO AL 953414-07-8

RX(44) RCT CJ 22253-71-0

STAGE(1)

RGT CN 7664-93-9 H2SO4, CO 7697-37-2 HNO3  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 4 hours, 125 deg C

STAGE(2)

RGT AP 7732-18-5 Water  
CON cooled

STAGE(3)

RGT AO 1310-73-2 NaOH  
SOL 7732-18-5 Water  
CON pH 7

PRO CM 147149-97-1

NTE regioselective, fuming nitric acid



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RX(43)     RCT   CM 147149-97-1  
             RGT   AU 1333-74-0 H2  
             PRO   AR 147149-98-2  
             CAT   7440-05-3 Pd  
             SOL   67-56-1 MeOH  
             CON   12 hours, room temperature  
             NTE   overall yield is 9% over two steps

RX(17)     RCT   AL 953414-07-8, AR 147149-98-2

             STAGE(1)

                 RGT   AO 1310-73-2 NaOH  
                 SOL   67-68-5 DMSO  
                 CON   SUBSTAGE(1) 80 deg C  
                             SUBSTAGE(2) 80 deg C -> 25 deg C

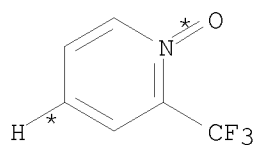
             STAGE(2)

                 RGT   AP 7732-18-5 Water  
                 CON   25 deg C

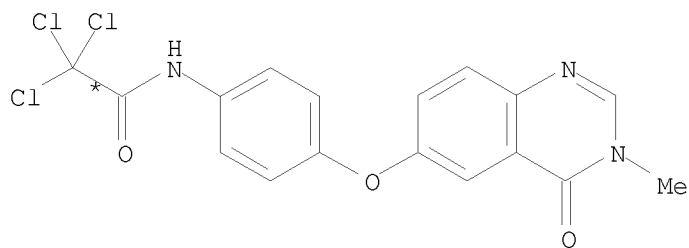
             PRO   AS 953414-04-5

RX(169) OF 215 COMPOSED OF RX(44), RX(43), RX(17)

RX(169)     CJ   +   AL   ==>   AS



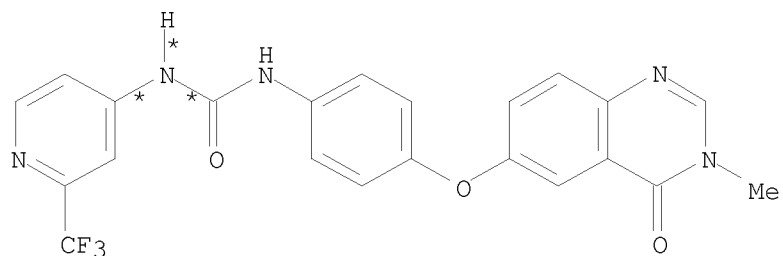
CJ



AL

3  
STEPS  
→

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AS

RX(44) RCT CJ 22253-71-0

STAGE(1)

RGT CN 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, CO 7697-37-2 HNO<sub>3</sub>

SOL 7732-18-5 Water

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 4 hours, 125 deg C

STAGE(2)

RGT AP 7732-18-5 Water

CON cooled

STAGE(3)

RGT AO 1310-73-2 NaOH

SOL 7732-18-5 Water

CON pH 7

PRO CM 147149-97-1

NTE regioselective, fuming nitric acid

RX(43) RCT CM 147149-97-1

RGT AU 1333-74-0 H<sub>2</sub>

PRO AR 147149-98-2

CAT 7440-05-3 Pd

SOL 67-56-1 MeOH

CON 12 hours, room temperature

NTE overall yield is 9% over two steps

RX(17) RCT AL 953414-07-8, AR 147149-98-2

STAGE(1)

RGT AO 1310-73-2 NaOH

SOL 67-68-5 DMSO

CON SUBSTAGE(1) 80 deg C

SUBSTAGE(2) 80 deg C -> 25 deg C

STAGE(2)

RGT AP 7732-18-5 Water

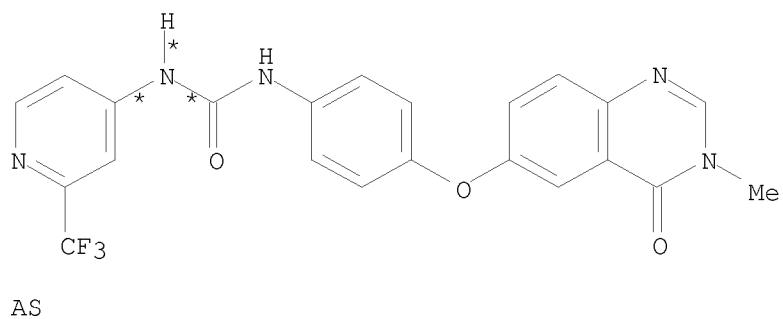
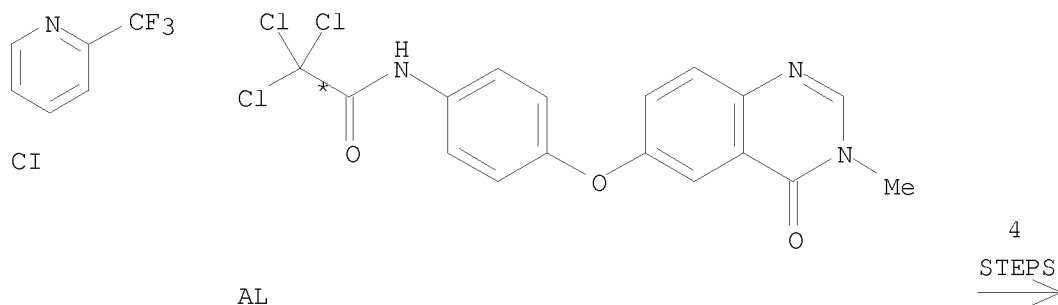
CON 25 deg C

PRO AS 953414-04-5

RX(170) OF 215 COMPOSED OF RX(42), RX(44), RX(43), RX(17)

RX(170) CI + AL ==> AS

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RX(42) RCT CI 368-48-9

STAGE(1)

RGT CK 937-14-4 MCPBA  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 12 hours, 25 deg C

STAGE(2)

RGT CL 144-55-8 NaHCO<sub>3</sub>  
SOL 7732-18-5 Water

PRO CJ 22253-71-0

RX(44) RCT CJ 22253-71-0

STAGE(1)

RGT CN 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, CO 7697-37-2 HNO<sub>3</sub>  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 4 hours, 125 deg C

STAGE(2)

RGT AP 7732-18-5 Water  
CON cooled

STAGE(3)

RGT AO 1310-73-2 NaOH  
SOL 7732-18-5 Water  
CON pH 7

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PRO CM 147149-97-1  
NTE regioselective, fuming nitric acid

RX(43) RCT CM 147149-97-1  
RGT AU 1333-74-0 H2  
PRO AR 147149-98-2  
CAT 7440-05-3 Pd  
SOL 67-56-1 MeOH  
CON 12 hours, room temperature  
NTE overall yield is 9% over two steps

RX(17) RCT AL 953414-07-8, AR 147149-98-2

STAGE(1)

RGT AO 1310-73-2 NaOH  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 80 deg C  
SUBSTAGE(2) 80 deg C -> 25 deg C

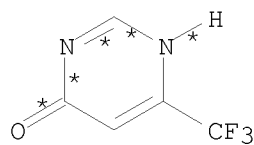
STAGE(2)

RGT AP 7732-18-5 Water  
CON 25 deg C

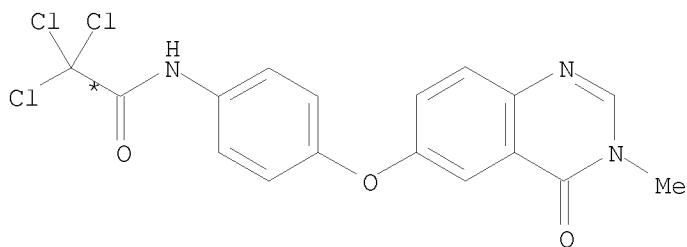
PRO AS 953414-04-5

RX(176) OF 215 COMPOSED OF RX(50), RX(23), RX(16)

RX(176) DE + AL ==> AN



DE



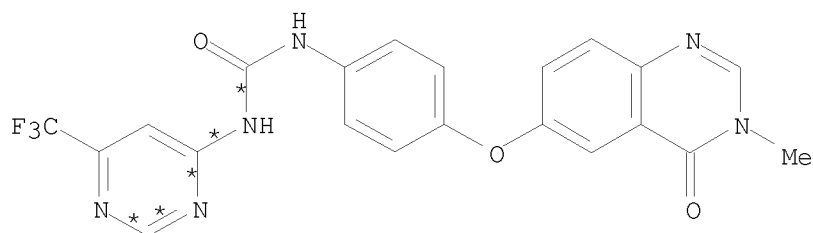
AL

3

STEPS



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AN  
YIELD 35%

RX(50) RCT DE 1546-78-7  
RGT DF 824-72-6 PhP(O)Cl2  
PRO BH 37552-81-1  
CON SUBSTAGE(1) 30 minutes, 130 deg C  
SUBSTAGE(2) 130 deg C -> 25 deg C

RX(23) RCT BH 37552-81-1  
RGT BI 7664-41-7 NH3  
PRO AM 672-41-3  
SOL 67-56-1 MeOH  
CON 12 hours, 25 deg C  
NTE overall yield is 29% over two steps

RX(16) RCT AL 953414-07-8, AM 672-41-3

STAGE(1)

RGT AO 1310-73-2 NaOH  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 80 deg C  
SUBSTAGE(2) 80 deg C -> 25 deg C

STAGE(2)

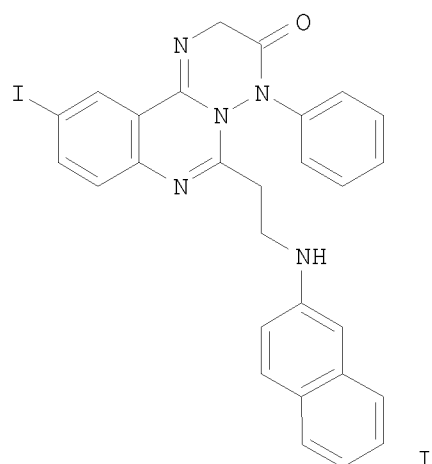
RGT AP 7732-18-5 Water  
CON 25 deg C

PRO AN 953414-03-4

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

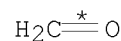
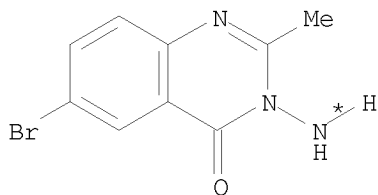
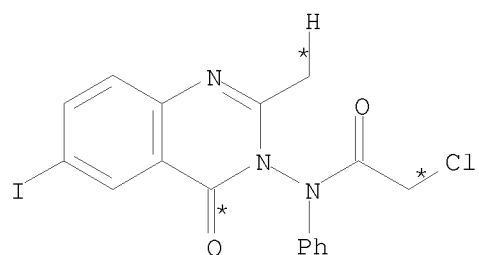
L3 ANSWER 10 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 147:448747 CASREACT  
TITLE: Synthesis, insecticidal and antimicrobial activities  
of some heterocyclic derivatives of quinazolinone  
AUTHOR(S): Singh, Tripti; Sharma, Shalabh; Srivastava, Virendra  
Kishore; Kumar, Ashok  
CORPORATE SOURCE: Medicinal Chemistry Division, Department of  
Pharmacology, Lala Lajpat Rai Memorial Medical  
College, Meerut, 250 004, India  
SOURCE: Indian Journal of Chemistry, Section B: Organic  
Chemistry Including Medicinal Chemistry (2006),  
45B(11), 2558-2565

CODEN: IJSBDB; ISSN: 0376-4699  
 PUBLISHER: National Institute of Science Communication and  
 Information Resources  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



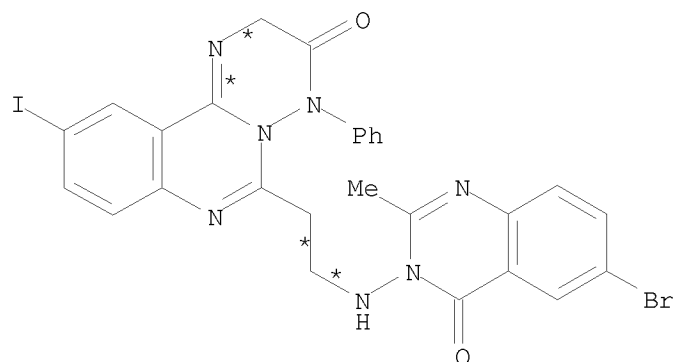
AB Some triazinoquinazoline derivs., e.g., I, have been synthesized from 4-phenyl-2,3-dihydro-6-methyl-10-iodo[1,2,3]-triazino[2,3-c]quinazolin-5-one by introducing aromatic nuclei via Mannich reaction with arylamines. These compds. were screened for insecticidal, anti-fungal and antibacterial activities. Compound I was found to be the most potent compound compared with the standard. Moreover, compound I also showed antibacterial activity. The structures of these compds. were elucidated by IR, <sup>1</sup>H NMR, mass spectroscopy and elemental anal.

RX(22) OF 69 COMPOSED OF RX(5), RX(9)  
 RX(22) M + X + R ==> Y



2  
 STEPS  
 →

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Y  
YIELD 45%

RX(5) RCT M 952430-81-8  
RGT P 631-61-8 NH4OAc  
PRO O 952430-82-9  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 8 hours, reflux

RX(9) RCT O 952430-82-9, X 71822-97-4, R 50-00-0  
RGT K 64-17-5 EtOH  
PRO Y 952430-85-2  
CON 8 hours, reflux  
NTE Mannich reaction

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 147:448727 CASREACT

TITLE: Synthesis of 2-methyl-3-tolyl-4-quinazolinone hydrochloride

AUTHOR(S): Zeng, Guiping; Sun, Fuqiang

CORPORATE SOURCE: College of Pharmaceutical Science, Guangdong College of Pharmacy, Guangzhou, 510224, Peop. Rep. China

SOURCE: Huaxue Shijie (2005), 46(12), 732-733, 725  
CODEN: HUAKAB; ISSN: 0367-6358

PUBLISHER: Shanghaishi Huaxue Huagong Xuehui

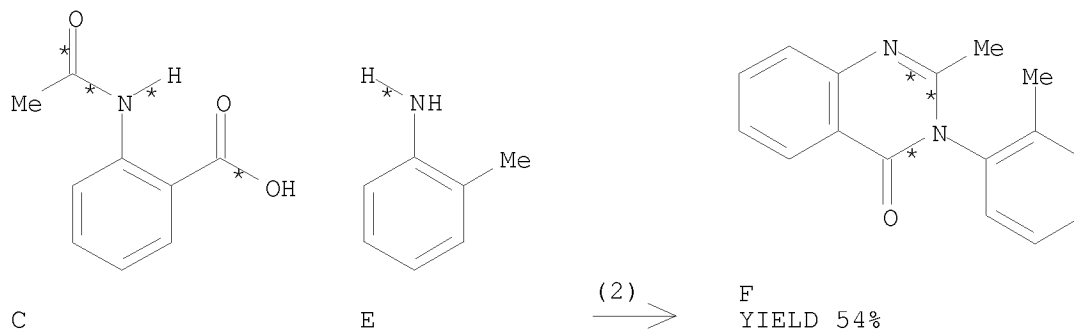
DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB ; -Methyl-3-(methylphenyl)-4-quinazolinone hydrochloride was prepared from anthranilic acid by condensation with acetic anhydride, cyclization with o-methylaniline or p-methylaniline in the presence of a dehydration agent (POCl<sub>3</sub>, H<sub>2</sub>SO<sub>4</sub>, P<sub>2</sub>O<sub>5</sub>) and salt formation with HCl. The compds. thus prepared included methaqualone hydrochloride [i.e., 2-methyl-3-(2-methylphenyl)-4(3H)-quinazolinone hydrochloride] and 2-methyl-3-(4-methylphenyl)-4(3H)-quinazolinone hydrochloride.

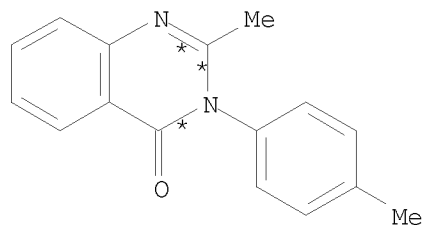
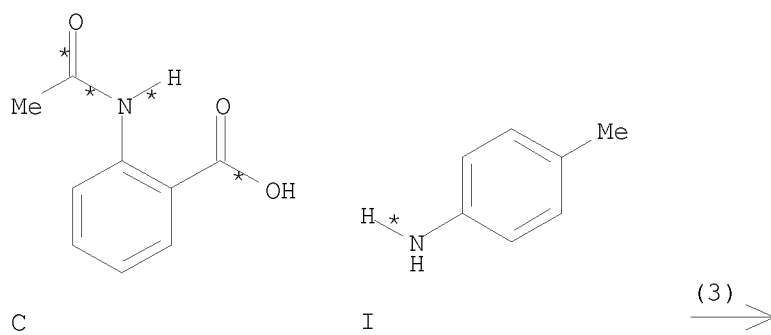
RX(2) OF 9 ...C + E ==> F

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RX(2) RCT C 89-52-1, E 95-53-4  
RGT G 10025-87-3 POC13  
PRO F 72-44-6  
SOL 108-88-3 PhMe  
CON 1.5 hours, reflux  
NTE optimization study, optimized on reaction time

RX(3) OF 9 ...C + I ==> J



J  
YIELD 40%

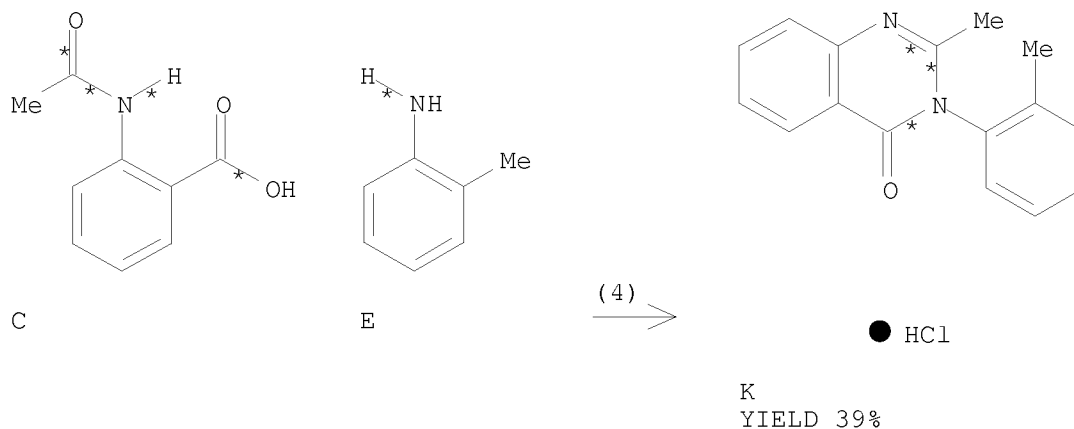
RX(3) RCT C 89-52-1, I 106-49-0  
RGT G 10025-87-3 POC13  
PRO J 22316-59-2  
SOL 108-88-3 PhMe



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CON 1.5 hours, reflux  
NTE optimization study, optimized on reaction time

RX(4) OF 9 ...C + E ==> K



RX(4) RCT C 89-52-1, E 95-53-4

STAGE(1)

RGT G 10025-87-3 POC13  
SOL 108-88-3 PhMe  
CON 1.5 hours, reflux

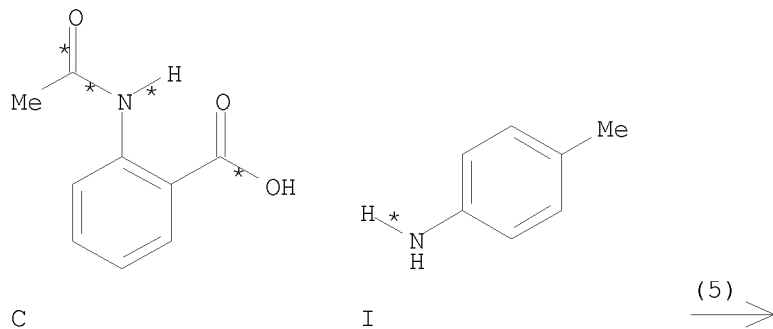
STAGE(2)

RGT L 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON heated

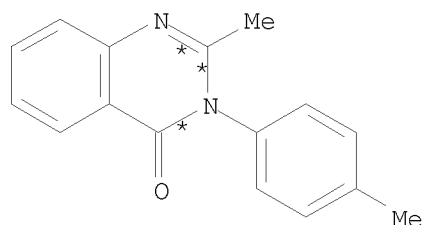
PRO K 340-56-7

NTE optimization study, optimized on reagent

RX(5) OF 9 ...C + I ==> M



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● HCl

M  
YIELD 56%

RX(5) RCT C 89-52-1, I 106-49-0

STAGE(1)

RGT G 10025-87-3 POC13  
SOL 108-88-3 PhMe  
CON 1.5 hours, reflux

STAGE(2)

RGT L 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON heated

PRO M 80257-03-0

NTE optimization study, optimized on reagent

L3 ANSWER 12 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 147:406780 CASREACT

TITLE: Synthesis of 7-bromo-6-chloro-4-quinazolinone and  
5-bromo-6-chloro-4-quinazolinone

AUTHOR(S): Zhang, Yue; Niu, Yuhuan; Dong, Bofang; Wang, Yinhua;  
Di, Xiaotao; Du, Huiru

CORPORATE SOURCE: Chemical and Pharmaceutical Engineering College, Hebei  
University of Science and Technology, Shijiazhuang,  
Hebei Province, 050018, Peop. Rep. China

SOURCE: Jingxi Huagong (2006), 23(8), 822-824  
CODEN: JIHUFJ; ISSN: 1003-5214

PUBLISHER: Jingxi Huagong Bianjibu

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

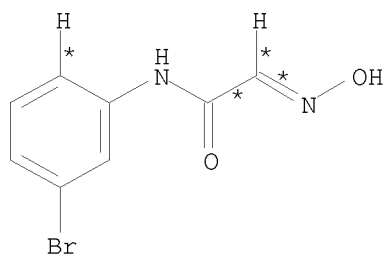
AB N-(3-Bromophenyl)-2-(hydroxyimino)acetamide was synthesized from  
m-bromoaniline and chloral hydrate in 90.5% yield. By treatment with  
concentrated sulfuric acid this compound cyclized to give a mixture of  
6-bromoisatin  
and 4-bromoisatin in 97.6% yield. Chlorination of bromoisatin gave  
6-bromo-5-chloroisatin in 86.8% yield and acetic acid was used as solvent  
instead of toxic nitrobenzene. The latter compound was oxidized by aqueous  
hydrogen peroxide to form 2-amino-4-bromo-5-chlorobenzoic acid. Treatment

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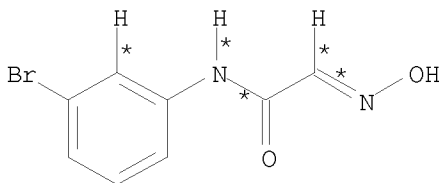
with phosphorous oxychloride and formamide gave  
7-bromo-6-chloro-4(3H)-quinazolinone. The total yield was 12.14%.  
5-Bromo-6-chloro-4(3H)-quinazolinone was synthesized in the same way and  
the total yield was 13.47%.

RX(26) OF 28 COMPOSED OF RX(2), RX(7), RX(8), RX(9)

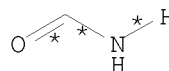
RX(26) 2 C + R ==> W



C

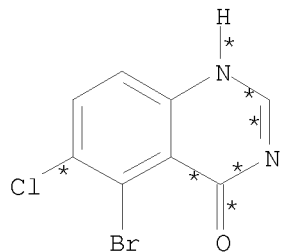


C



R

4  
STEPS  
→



W  
YIELD 65%

RX(2) RCT C 65971-74-6

STAGE(1)

RGT E 7664-93-9 H2SO4

SOL 7732-18-5 Water

CON SUBSTAGE(1) room temperature -> 50 deg C

SUBSTAGE(2) 50 deg C

SUBSTAGE(3) 0.5 hours, 70 - 75 deg C

SUBSTAGE(4) 75 deg C -> room temperature

STAGE(2)

RGT G 7732-18-5 Water

CON 0.5 hours, cooled

STAGE(3)

RGT J 1310-73-2 NaOH

SOL 7732-18-5 Water  
CON room temperature

STAGE(4)

RGT E 7664-93-9 H<sub>2</sub>SO<sub>4</sub>  
SOL 7732-18-5 Water  
CON room temperature, pH 8

STAGE(5)

RGT K 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, pH 3.5

PRO H 6326-79-0, I 20780-72-7

RX(7)

RCT I 20780-72-7  
RGT O 64-19-7 AcOH, M 7719-09-7 SOCl<sub>2</sub>, N 7791-25-5 SO<sub>2</sub>Cl<sub>2</sub>  
PRO U 65971-75-7  
CON SUBSTAGE(1) room temperature -> 80 deg C  
SUBSTAGE(2) 80 - 85 deg C  
SUBSTAGE(3) 85 deg C -> 90 deg C  
SUBSTAGE(4) 45 minutes, 85 - 95 deg C  
SUBSTAGE(5) 95 deg C -> room temperature  
NTE catalyst used

RX(8)

RCT U 65971-75-7  
STAGE(1)  
RGT J 1310-73-2 NaOH, Q 7722-84-1 H<sub>2</sub>O<sub>2</sub>  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 20 minutes, room temperature  
SUBSTAGE(2) 45 minutes, room temperature

STAGE(2)

RGT K 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, acidify

PRO V 65971-76-8

RX(9)

RCT R 75-12-7, V 65971-76-8  
STAGE(1)  
RGT T 10025-87-3 POCl<sub>3</sub>  
CON SUBSTAGE(1) room temperature -> 90 deg C  
SUBSTAGE(2) 90 - 95 deg C  
SUBSTAGE(3) 30 minutes, 90 - 95 deg C  
SUBSTAGE(4) cooled  
STAGE(2)  
RGT G 7732-18-5 Water  
CON cooled  
PRO W 65971-77-9  
NTE 13% overall yield from 3-bromo-Benzenamine

L3 ANSWER 13 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 147:344042 CASREACT

TITLE: Synthesis of new 4(3H)-quinazolinone derivatives

AUTHOR(S): Truong, The Ky; Nguyen, Anh Tuan; Ly, Da Thoi; Pham, Khanh Phong Lan

CORPORATE SOURCE: Dept. Pharmacy, Ho Chi Minh City College of Pharmacy and Medicine, Vietnam

SOURCE: Tap Chi Hoa Hoc (2006), 44(4), 445-448

CODEN: TCHHDC; ISSN: 0378-2336

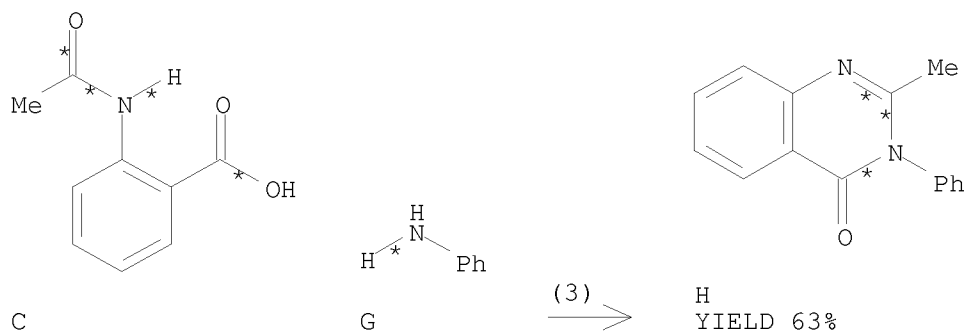
PUBLISHER: Toa Soan Tap Chi Hoa Hoc

DOCUMENT TYPE: Journal

LANGUAGE: Vietnamese

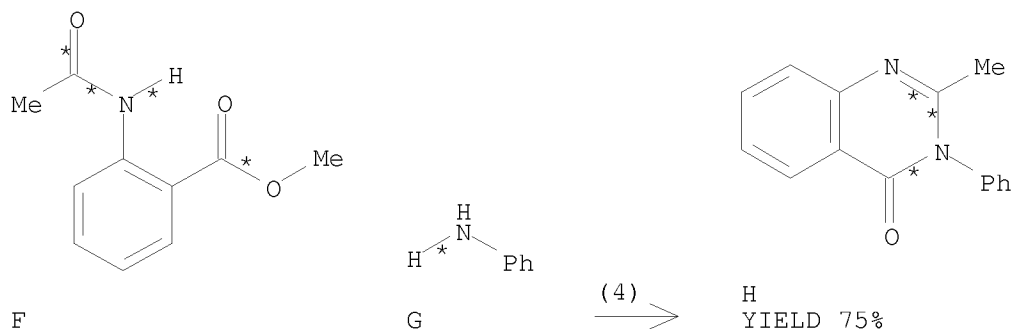
AB For the pharmacomodulation of 4(3H)-quinazolinone, a heterocycle with many advantages in therapy, the authors implemented nucleophilic substitution on the chloromethyl group of position 2 using phenol and amine derivs. to give new compds. that showed potential antifungal and antibacterial activities. One antibacterial and antifungal triazolylmethylquinazolinone derivative synthesized in this research project showed MIC of 16  $\mu\text{g/mL}$  against *Candida albicans*.

RX(3) OF 70 ...C + G ==&gt; H...



RX(3) RCT C 89-52-1, G 62-53-3  
 PRO H 2385-23-1  
 NTE alternative preparation shown

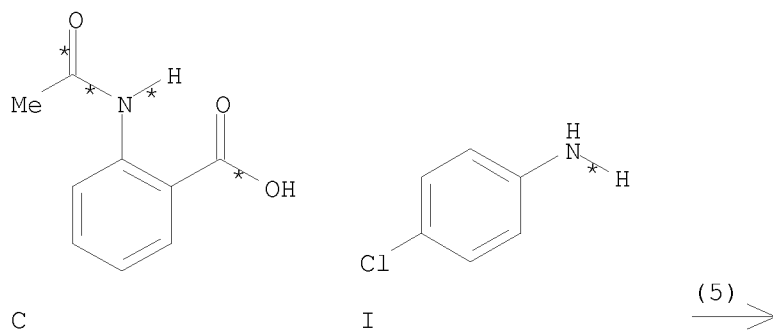
RX(4) OF 70 ...F + G ==&gt; H...



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RX(4) RCT F 2719-08-6, G 62-53-3  
PRO H 2385-23-1  
NTE alternative preparation shown

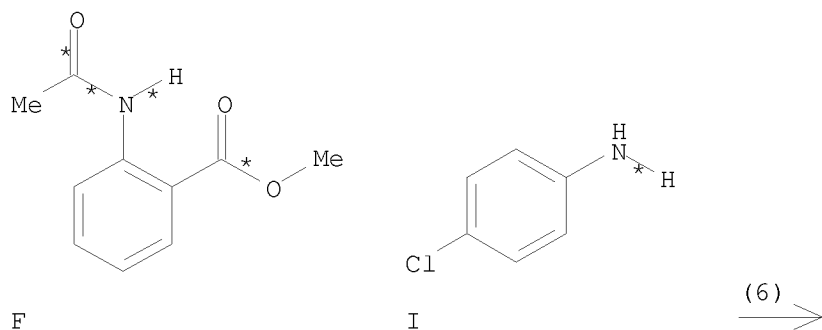
RX(5) OF 70 ...C + I ==> J...



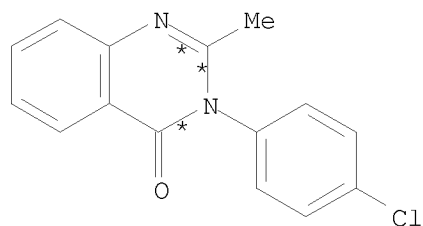
J  
YIELD 74%

RX(5) RCT C 89-52-1, I 106-47-8  
PRO J 1788-93-8  
NTE alternative preparation shown

RX(6) OF 70 ...F + I ==> J...



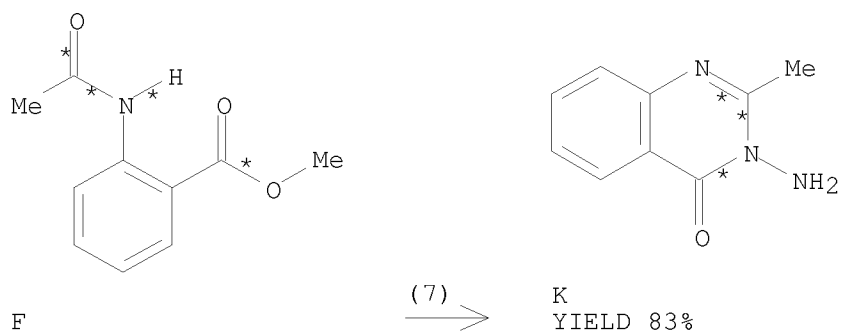
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J  
YIELD 87%

RX(6) RCT F 2719-08-6, I 106-47-8  
PRO J 1788-93-8  
NTE alternative preparation shown

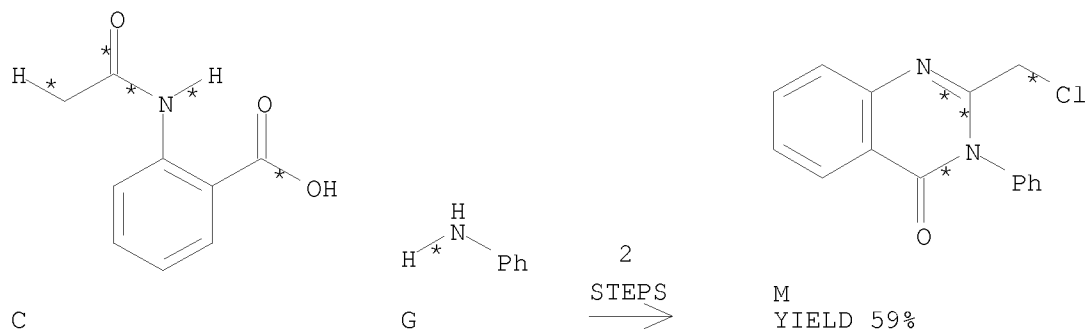
RX(7) OF 70 ...F ==> K



RX(7) RCT F 2719-08-6  
RGT L 302-01-2 N2H4  
PRO K 1898-06-2

RX(23) OF 70 COMPOSED OF RX(3), RX(8)  
RX(23) C + G ==> M

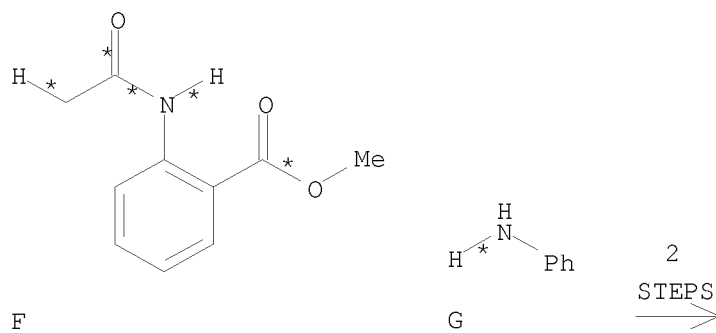
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RX(3) RCT C 89-52-1, G 62-53-3  
PRO H 2385-23-1  
NTE alternative preparation shown

RX(8) RCT H 2385-23-1  
RGT N 128-08-5 Bromosuccinimide  
PRO M 22312-77-2  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl3

RX(24) OF 70 COMPOSED OF RX(4), RX(8)  
RX(24) F + G ==> M



RX(4) RCT F 2719-08-6, G 62-53-3



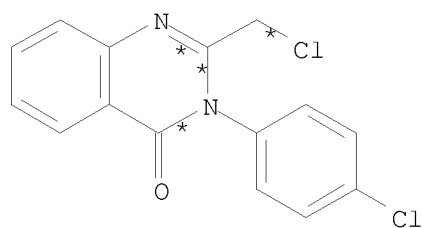
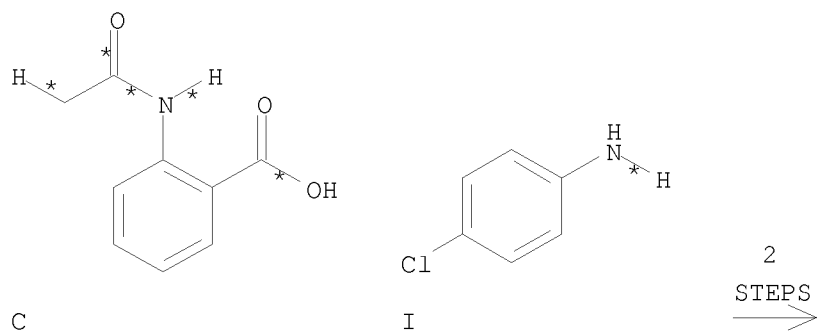
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PRO H 2385-23-1  
NTE alternative preparation shown

RX(8) RCT H 2385-23-1  
RGT N 128-08-5 Bromosuccinimide  
PRO M 22312-77-2  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl<sub>3</sub>

RX(25) OF 70 COMPOSED OF RX(5), RX(9)

RX(25) C + I ==> Q



Q  
YIELD 53%

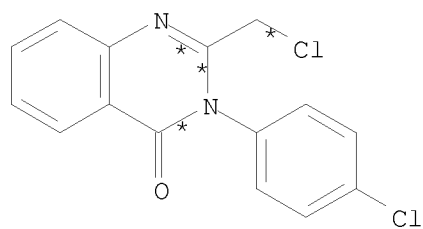
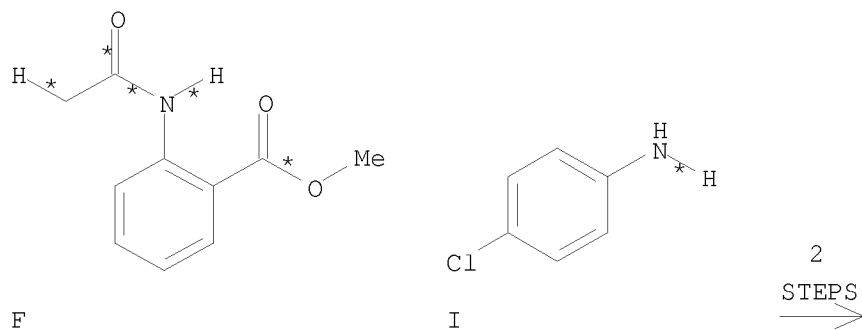
RX(5) RCT C 89-52-1, I 106-47-8  
PRO J 1788-93-8  
NTE alternative preparation shown

RX(9) RCT J 1788-93-8  
RGT N 128-08-5 Bromosuccinimide  
PRO Q 22280-87-1  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl<sub>3</sub>

RX(26) OF 70 COMPOSED OF RX(6), RX(9)

RX(26) F + I ==> Q

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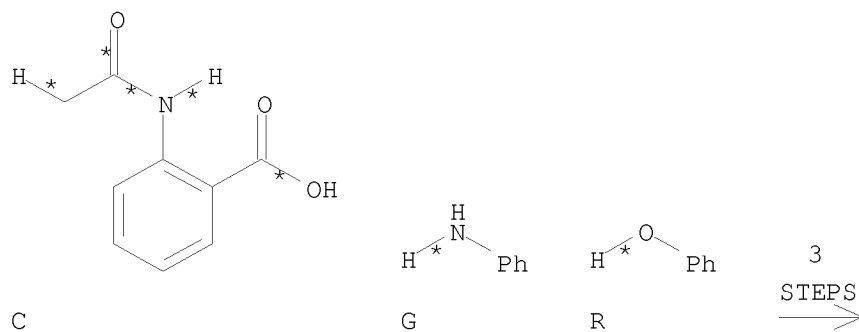


Q  
YIELD 53%

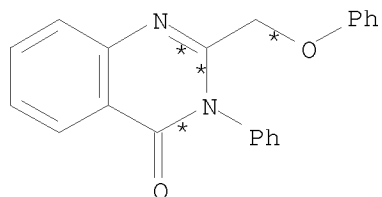
RX(6) RCT F 2719-08-6, I 106-47-8  
PRO J 1788-93-8  
NTE alternative preparation shown

RX(9) RCT J 1788-93-8  
RGT N 128-08-5 Bromosuccinimide  
PRO Q 22280-87-1  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl<sub>3</sub>

RX(39) OF 70 COMPOSED OF RX(3), RX(8), RX(10)  
RX(39) C + G + R ==> S



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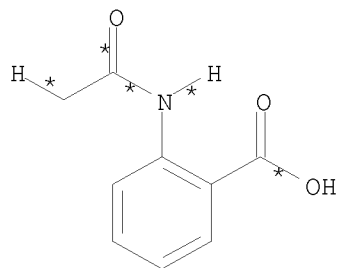
S  
YIELD 39%

RX(3) RCT C 89-52-1, G 62-53-3  
PRO H 2385-23-1  
NTE alternative preparation shown

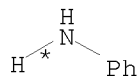
RX(8) RCT H 2385-23-1  
RGT N 128-08-5 Bromosuccinimide  
PRO M 22312-77-2  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl3

RX(10) RCT M 22312-77-2, R 108-95-2  
RGT T 1310-73-2 NaOH  
PRO S 20873-22-7  
SOL 68-12-2 DMF  
NTE Williamson reaction

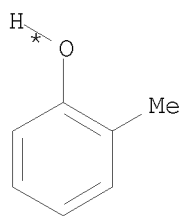
RX(40) OF 70 COMPOSED OF RX(3), RX(8), RX(11)  
RX(40) C + G + V ==> W



C



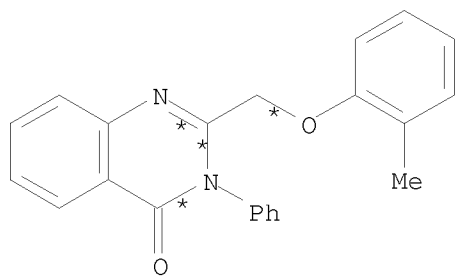
G



V

3  
STEPS  
→

10/ 562,112



W  
YIELD 23%

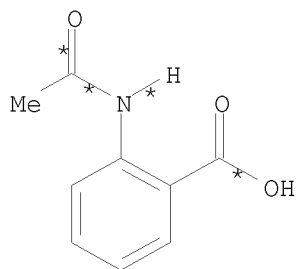
RX(3) RCT C 89-52-1, G 62-53-3  
PRO H 2385-23-1  
NTE alternative preparation shown

RX(8) RCT H 2385-23-1  
RGT N 128-08-5 Bromosuccinimide  
PRO M 22312-77-2  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl<sub>3</sub>

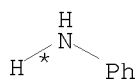
RX(11) RCT M 22312-77-2, V 95-48-7  
RGT T 1310-73-2 NaOH  
PRO W 948312-75-2  
SOL 68-12-2 DMF  
NTE Williamson reaction

RX(41) OF 70 COMPOSED OF RX(3), RX(8), RX(12)

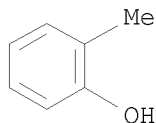
RX(41) C + G + V ==> X



C



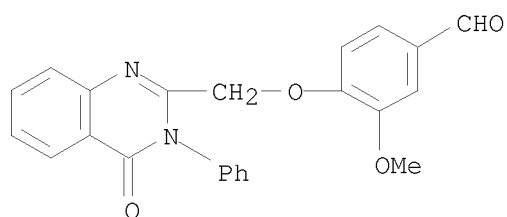
G



V

3  
STEPS  
→

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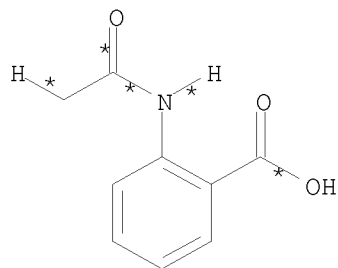
X  
YIELD 22%

RX(3) RCT C 89-52-1, G 62-53-3  
PRO H 2385-23-1  
NTE alternative preparation shown

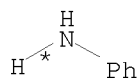
RX(8) RCT H 2385-23-1  
RGT N 128-08-5 Bromosuccinimide  
PRO M 22312-77-2  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl3

RX(12) RCT M 22312-77-2, V 95-48-7  
RGT T 1310-73-2 NaOH  
PRO X 948312-76-3  
SOL 68-12-2 DMF  
NTE Williamson reaction, an unspecified acetal of vanilin used

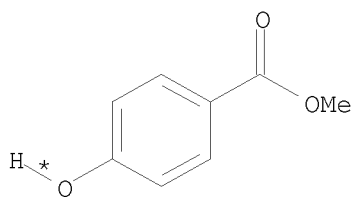
RX(42) OF 70 COMPOSED OF RX(3), RX(8), RX(13)  
RX(42) C + G + Y ==> Z



C



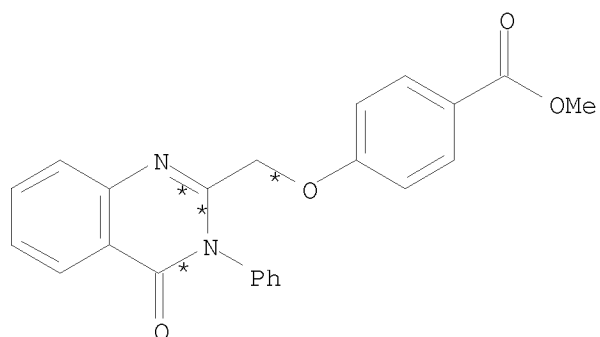
G



Y

3  
STEPS  
→

10/ 562,112



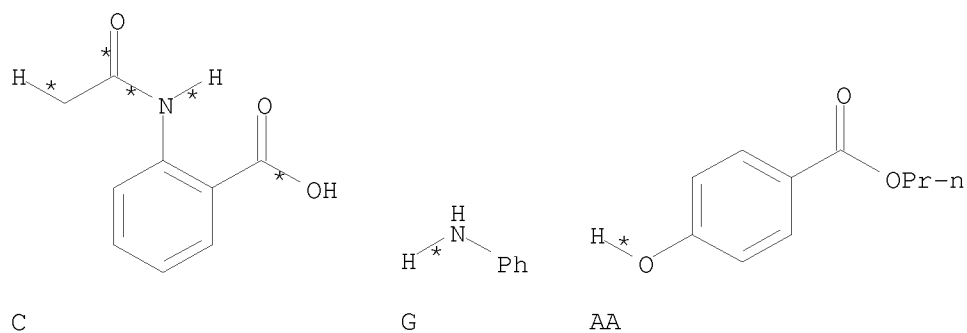
Z  
YIELD 33%

RX(3) RCT C 89-52-1, G 62-53-3  
PRO H 2385-23-1  
NTE alternative preparation shown

RX(8) RCT H 2385-23-1  
RGT N 128-08-5 Bromosuccinimide  
PRO M 22312-77-2  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl3

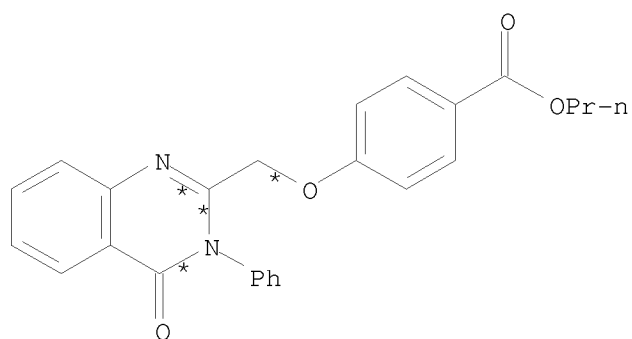
RX(13) RCT M 22312-77-2, Y 99-76-3  
RGT T 1310-73-2 NaOH  
PRO Z 948312-77-4  
SOL 68-12-2 DMF  
NTE Williamson reaction

RX(43) OF 70 COMPOSED OF RX(3), RX(8), RX(14)  
RX(43) C + G + AA ==> AB



3  
STEPS  
→

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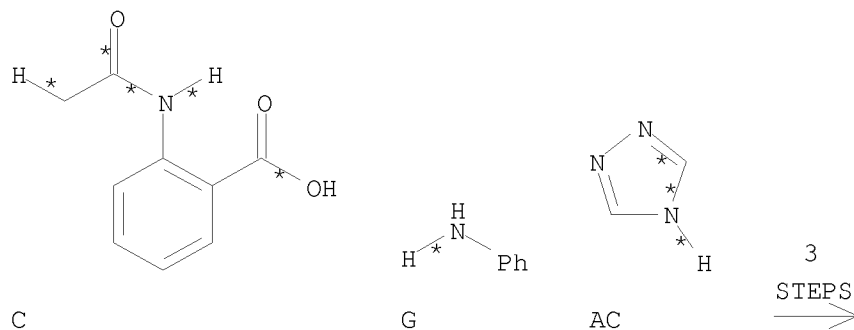
AB  
YIELD 29%

RX(3) RCT C 89-52-1, G 62-53-3  
PRO H 2385-23-1  
NTE alternative preparation shown

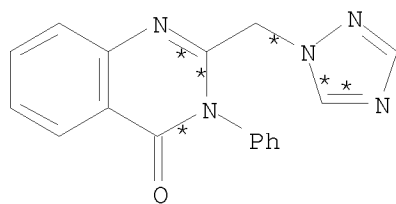
RX(8) RCT H 2385-23-1  
RGT N 128-08-5 Bromosuccinimide  
PRO M 22312-77-2  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl3

RX(14) RCT M 22312-77-2, AA 94-13-3  
RGT T 1310-73-2 NaOH  
PRO AB 948312-78-5  
SOL 68-12-2 DMF  
NTE Williamson reaction

RX(44) OF 70 COMPOSED OF RX(3), RX(8), RX(15)  
RX(44) C + G + AC ==> AD



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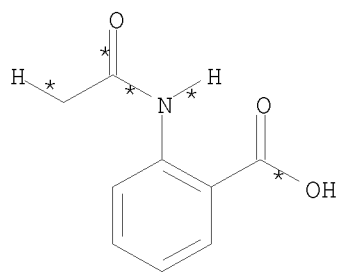
AD  
YIELD 31%

RX(3) RCT C 89-52-1, G 62-53-3  
PRO H 2385-23-1  
NTE alternative preparation shown

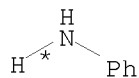
RX(8) RCT H 2385-23-1  
RGT N 128-08-5 Bromosuccinimide  
PRO M 22312-77-2  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl3

RX(15) RCT M 22312-77-2, AC 288-88-0  
PRO AD 948312-72-9  
CAT 7440-23-5 Na  
SOL 67-56-1 MeOH

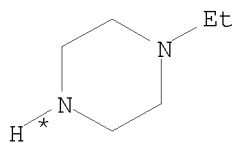
RX(45) OF 70 COMPOSED OF RX(3), RX(8), RX(16)  
RX(45) C + G + AG ==> AH



C

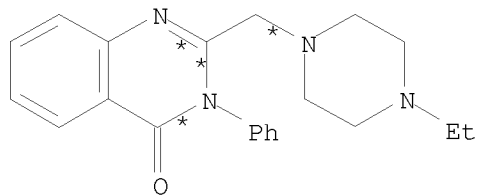


G



AG

3  
STEPS  
→



AH  
YIELD 24%



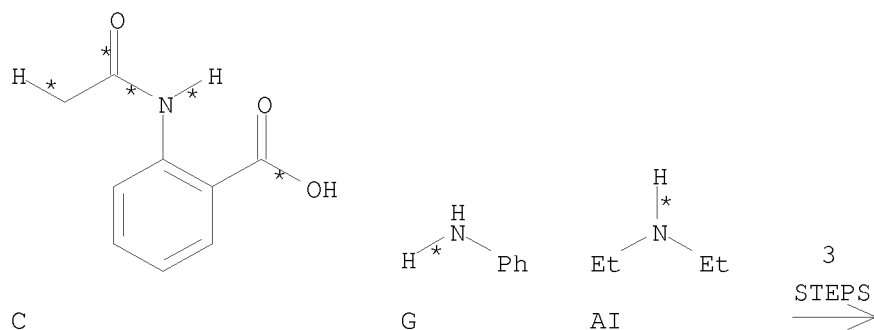
10/ 562,112

RX(3)      RCT    C 89-52-1, G 62-53-3  
            PRO    H 2385-23-1  
            NTE    alternative preparation shown

RX(8)      RCT    H 2385-23-1  
            RGT    N 128-08-5 Bromosuccinimide  
            PRO    M 22312-77-2  
            CAT    110-86-1 Pyridine  
            SOL    67-66-3 CHCl<sub>3</sub>

RX(16)     RCT    M 22312-77-2, AG 5308-25-8  
            PRO    AH 948312-73-0  
            CAT    7440-23-5 Na  
            SOL    67-56-1 MeOH

RX(46) OF 70 COMPOSED OF RX(3), RX(8), RX(17)  
RX(46)      C    +    G    +    AI    ==>    AJ



AJ  
YIELD 40%

RX(3)      RCT    C 89-52-1, G 62-53-3  
            PRO    H 2385-23-1  
            NTE    alternative preparation shown

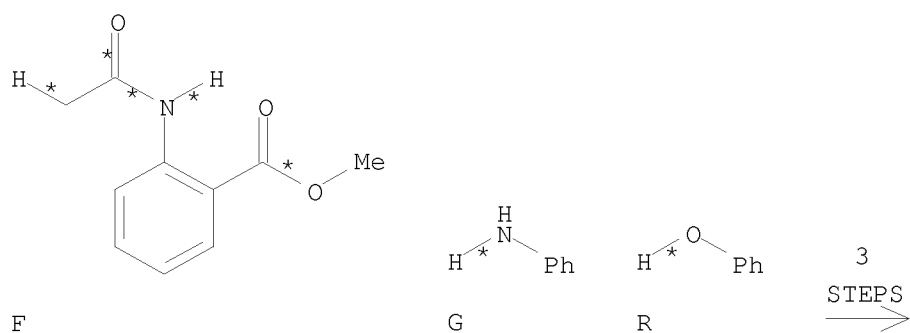
RX(8)      RCT    H 2385-23-1  
            RGT    N 128-08-5 Bromosuccinimide  
            PRO    M 22312-77-2

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CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl<sub>3</sub>

RX(17) RCT M 22312-77-2, AI 109-89-7  
PRO AJ 948312-74-1  
CAT 7440-23-5 Na  
SOL 67-56-1 MeOH

RX(47) OF 70 COMPOSED OF RX(4), RX(8), RX(10)  
RX(47) F + G + R ==> S



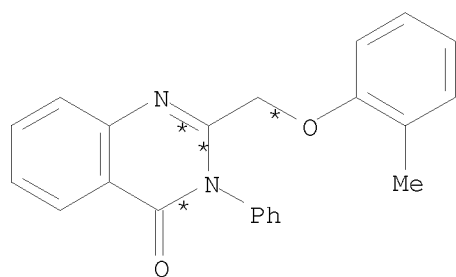
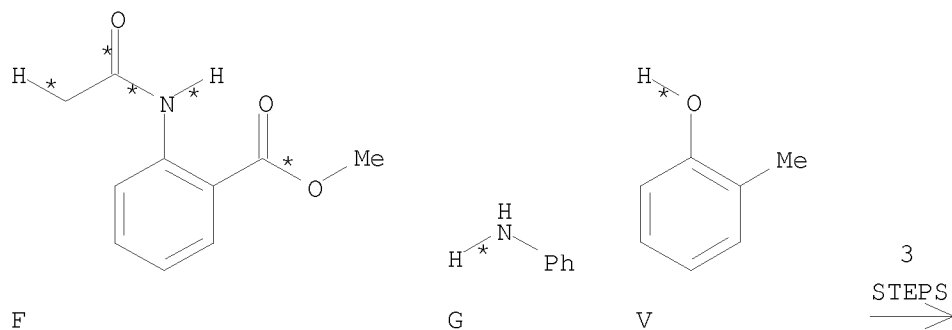
S  
YIELD 39%

RX(4) RCT F 2719-08-6, G 62-53-3  
PRO H 2385-23-1  
NTE alternative preparation shown

RX(8) RCT H 2385-23-1  
RGT N 128-08-5 Bromosuccinimide  
PRO M 22312-77-2  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl<sub>3</sub>

RX(10) RCT M 22312-77-2, R 108-95-2  
RGT T 1310-73-2 NaOH  
PRO S 20873-22-7  
SOL 68-12-2 DMF  
NTE Williamson reaction

RX(48) OF 70 COMPOSED OF RX(4), RX(8), RX(11)  
RX(48) F + G + V ==> W



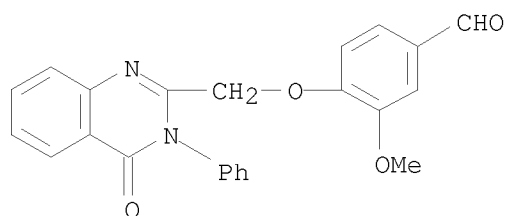
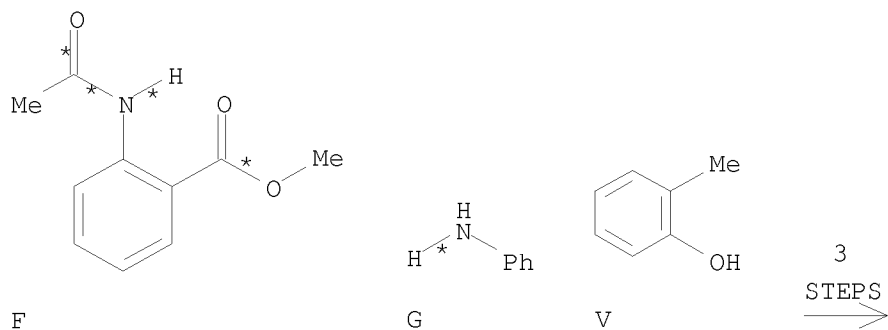
W  
YIELD 23%

RX(4) RCT F 2719-08-6, G 62-53-3  
PRO H 2385-23-1  
NTE alternative preparation shown

RX(8) RCT H 2385-23-1  
RGT N 128-08-5 Bromosuccinimide  
PRO M 22312-77-2  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl<sub>3</sub>

RX(11) RCT M 22312-77-2, V 95-48-7  
RGT T 1310-73-2 NaOH  
PRO W 948312-75-2  
SOL 68-12-2 DMF  
NTE Williamson reaction

RX(49) OF 70 COMPOSED OF RX(4), RX(8), RX(12)  
RX(49) F + G + V ==> X



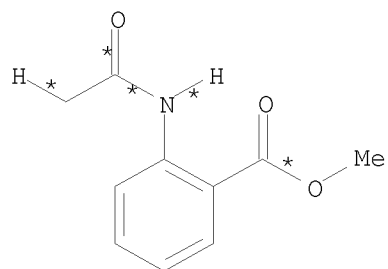
X  
YIELD 22%

RX(4) RCT F 2719-08-6, G 62-53-3  
PRO H 2385-23-1  
NTE alternative preparation shown

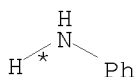
RX(8) RCT H 2385-23-1  
RGT N 128-08-5 Bromosuccinimide  
PRO M 22312-77-2  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl<sub>3</sub>

RX(12) RCT M 22312-77-2, V 95-48-7  
RGT T 1310-73-2 NaOH  
PRO X 948312-76-3  
SOL 68-12-2 DMF  
NTE Williamson reaction, an unspecified acetal of vanillin used

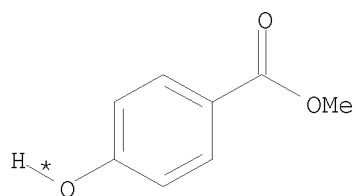
RX(50) OF 70 COMPOSED OF RX(4), RX(8), RX(13)  
RX(50) F + G + Y ==> Z



F

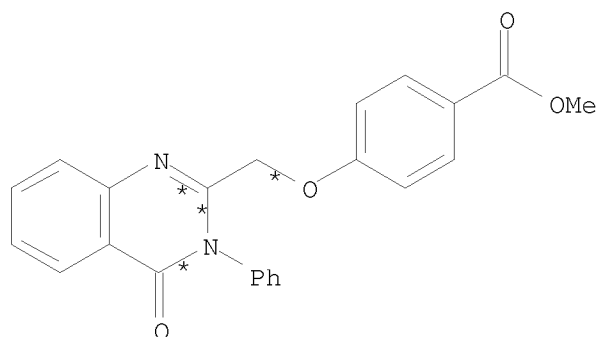


G



Y

3  
STEPS  
→



Z

YIELD 33%

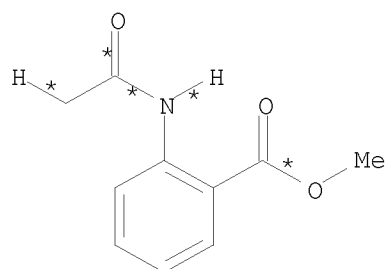
RX(4) RCT F 2719-08-6, G 62-53-3  
PRO H 2385-23-1  
NTE alternative preparation shown

RX(8) RCT H 2385-23-1  
RGT N 128-08-5 Bromosuccinimide  
PRO M 22312-77-2  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl3

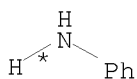
RX(13) RCT M 22312-77-2, Y 99-76-3  
RGT T 1310-73-2 NaOH  
PRO Z 948312-77-4  
SOL 68-12-2 DMF  
NTE Williamson reaction

RX(51) OF 70 COMPOSED OF RX(4), RX(8), RX(14)  
RX(51) F + G + AA ==> AB

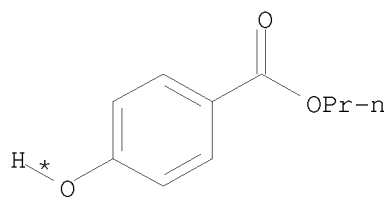
10/ 562,112



F

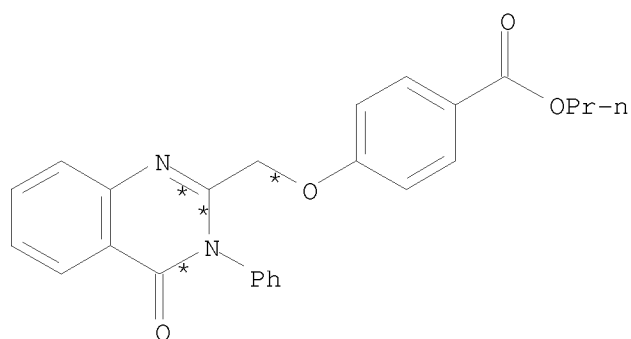


G



AA

3  
STEPS  
→



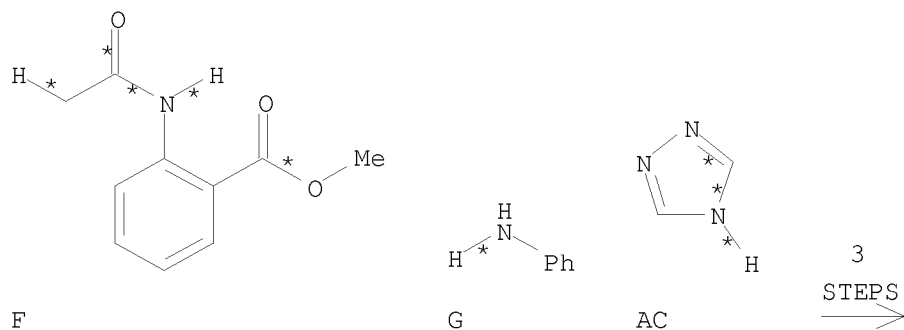
AB  
YIELD 29%

RX(4) RCT F 2719-08-6, G 62-53-3  
PRO H 2385-23-1  
NTE alternative preparation shown

RX(8) RCT H 2385-23-1  
RGT N 128-08-5 Bromosuccinimide  
PRO M 22312-77-2  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl3

RX(14) RCT M 22312-77-2, AA 94-13-3  
RGT T 1310-73-2 NaOH  
PRO AB 948312-78-5  
SOL 68-12-2 DMF  
NTE Williamson reaction

RX(52) OF 70 COMPOSED OF RX(4), RX(8), RX(15)  
RX(52) F + G + AC ==> AD



AD  
YIELD 31%

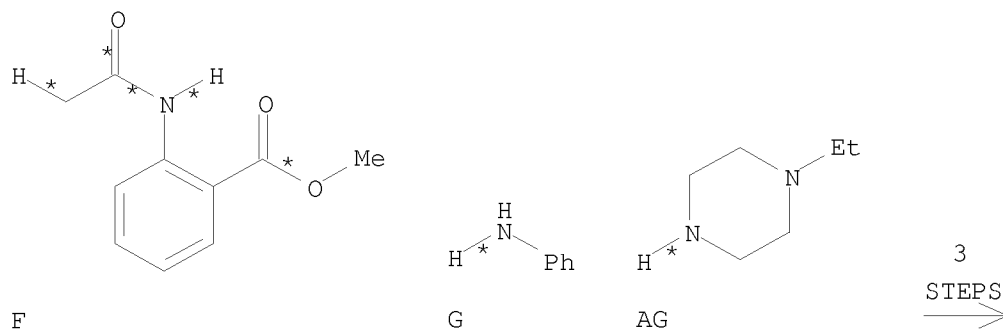
RX(4) RCT F 2719-08-6, G 62-53-3  
PRO H 2385-23-1  
NTE alternative preparation shown

RX(8) RCT H 2385-23-1  
RGT N 128-08-5 Bromosuccinimide  
PRO M 22312-77-2  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl<sub>3</sub>

RX(15) RCT M 22312-77-2, AC 288-88-0  
PRO AD 948312-72-9  
CAT 7440-23-5 Na  
SOL 67-56-1 MeOH

RX(53) OF 70 COMPOSED OF RX(4), RX(8), RX(16)

RX(53) F + G + AG ==> AH



AH  
YIELD 24%

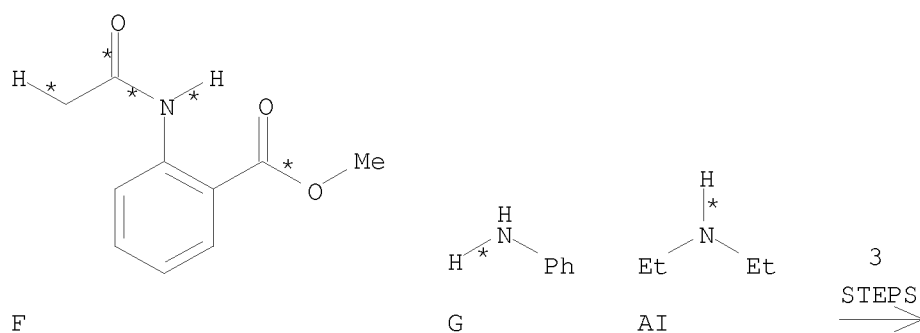
RX(4) RCT F 2719-08-6, G 62-53-3  
PRO H 2385-23-1  
NTE alternative preparation shown

RX(8) RCT H 2385-23-1  
RGT N 128-08-5 Bromosuccinimide  
PRO M 22312-77-2  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl<sub>3</sub>

RX(16) RCT M 22312-77-2, AG 5308-25-8  
PRO AH 948312-73-0  
CAT 7440-23-5 Na  
SOL 67-56-1 MeOH

RX(54) OF 70 COMPOSED OF RX(4), RX(8), RX(17)  
RX(54) F + G + AI ==> AJ





AJ  
YIELD 40%

RX(4) RCT F 2719-08-6, G 62-53-3  
PRO H 2385-23-1  
NTE alternative preparation shown

RX(8) RCT H 2385-23-1  
RGT N 128-08-5 Bromosuccinimide  
PRO M 22312-77-2  
CAT 110-86-1 Pyridine  
SOL 67-66-3 CHCl<sub>3</sub>

RX(17) RCT M 22312-77-2, AI 109-89-7  
PRO AJ 948312-74-1  
CAT 7440-23-5 Na  
SOL 67-56-1 MeOH

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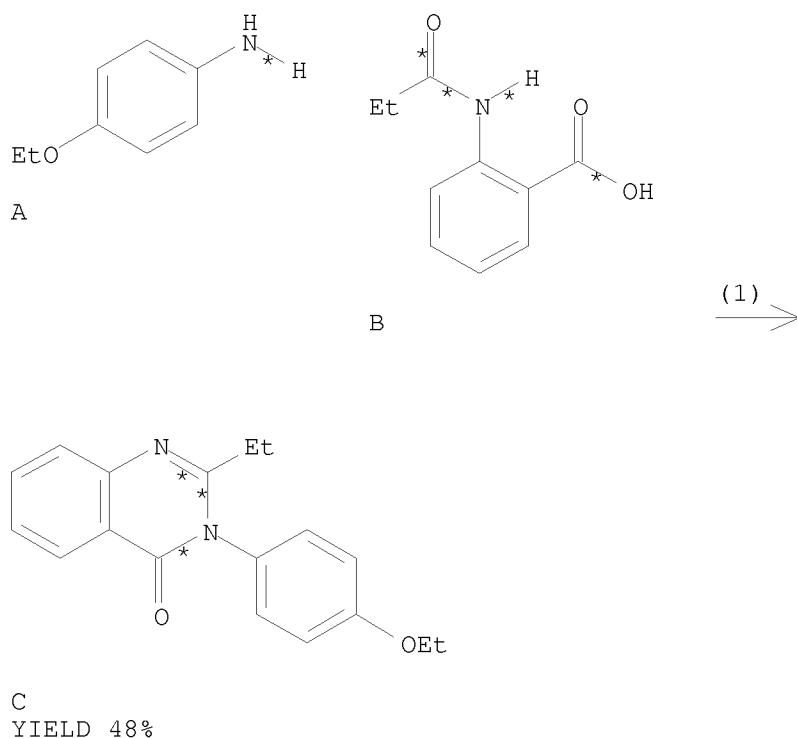
TITLE: Synthesis and structure-activity relationships of  
3H-quinazolin-4-ones and  
3H-pyrido[2,3-d]pyrimidin-4-ones as CXCR3 receptor  
antagonists

AUTHOR(S): Storelli, Stefania; Verzijl, Dennis; Al-Badie, Jawad;

CORPORATE SOURCE: Elders, Niels; Bosch, Leontien; Timmerman, Henk; Smit, Martine J.; De Esch, Iwan J. P.; Leurs, Rob  
 Leiden/Amsterdam Center for Drug Research (LACDR),  
 Division of Medicinal Chemistry, Faculty of Sciences,  
 Vrije Universiteit Amsterdam, Amsterdam, Neth.  
 SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2007),  
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 LANGUAGE: English

AB This study presents the synthesis and initial SAR of CXCR3 antagonists of the 3H-quinazolin-4-one and 3H-pyrido[2,3-d]pyrimidin-4-one series. These compds. as tools for targeting CXCR3 in a variety of inflammatory models are evaluated. Moreover, the structural insights obtained may be used in the design of novel CXCR3 antagonists.

RX(1) OF 112      ...A + B ==> C...



RX(1)      RCT    A 156-43-4, B 19165-26-5

STAGE(1)

RGT    D 7719-12-2 PC13

SOL    108-88-3 PhMe

CON    SUBSTAGE(1) room temperature -> reflux

         SUBSTAGE(2) 8 hours, reflux

         SUBSTAGE(3) reflux -> room temperature

STAGE(2)

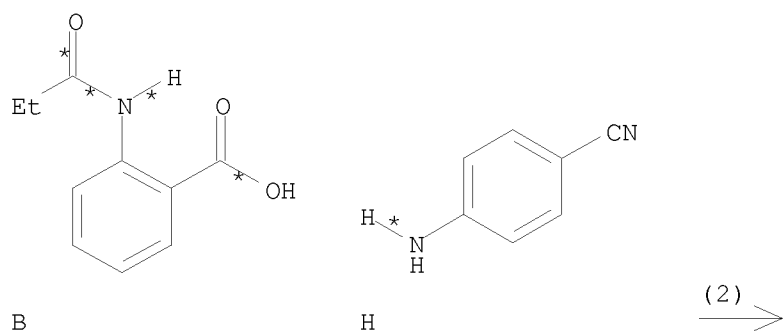
RGT    E 497-19-8 Na2CO3

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SOL 7732-18-5 Water  
CON room temperature

PRO C 93879-55-1

RX(2) OF 112 ...B + H ==> I...



I  
YIELD 35%

RX(2) RCT B 19165-26-5, H 873-74-5

STAGE(1)

RGT D 7719-12-2 PC13  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) room temperature -> reflux  
SUBSTAGE(2) 8 hours, reflux  
SUBSTAGE(3) reflux -> room temperature

STAGE(2)

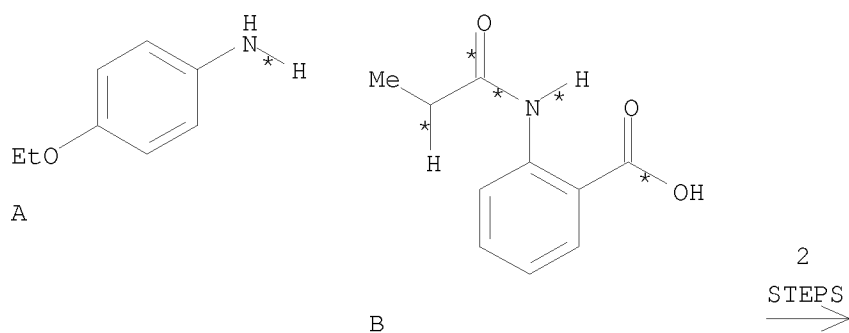
RGT E 497-19-8 Na2CO3  
SOL 7732-18-5 Water  
CON room temperature

PRO I 860002-79-5

RX(30) OF 112 COMPOSED OF RX(1), RX(4)

RX(30) A + B ==> M

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M  
YIELD 96%

RX(1) RCT A 156-43-4, B 19165-26-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

CON room temperature

PRO C 93879-55-1

RX(4)

RCT C 93879-55-1

RGT N 127-09-3 AcONa, O 7726-95-6 Br2

PRO M 876016-38-5

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) room temperature -> 40 deg C

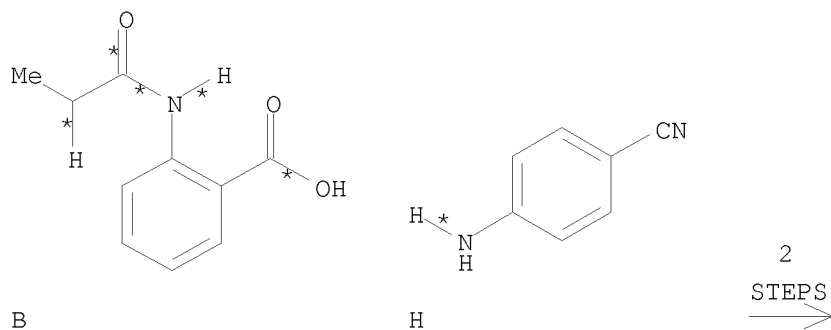
SUBSTAGE(2) 3 hours, 40 deg C

NTE regioselective

RX(31) OF 112 COMPOSED OF RX(2), RX(5)

RX(31) B + H ==> Q

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Q  
YIELD 88%

RX(2) RCT B 19165-26-5, H 873-74-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

CON room temperature

PRO I 860002-79-5

RX(5)

RCT I 860002-79-5

RGT N 127-09-3 AcONa, O 7726-95-6 Br2

PRO Q 860002-84-2

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) room temperature -> 40 deg C

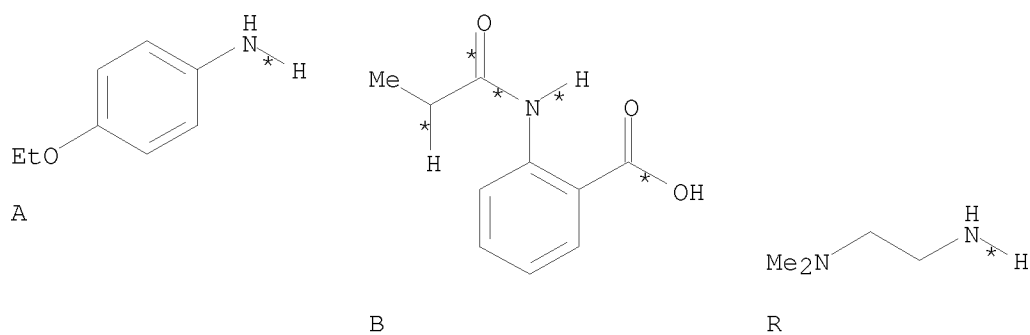
SUBSTAGE(2) 3 hours, 40 deg C

NTE regioselective

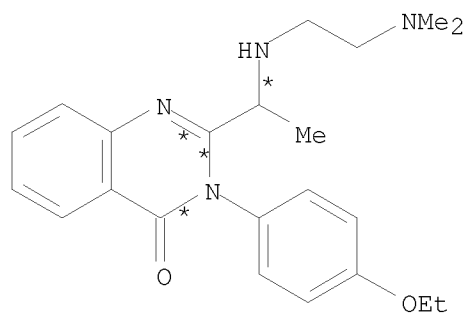
RX(57) OF 112 COMPOSED OF RX(1), RX(4), RX(6)

RX(57) A + B + R ==> S

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3  
STEPS  
→



S  
YIELD 52%

RX(1) RCT A 156-43-4, B 19165-26-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

CON room temperature

PRO C 93879-55-1

RX(4) RCT C 93879-55-1

RGT N 127-09-3 AcONa, O 7726-95-6 Br2

PRO M 876016-38-5

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) room temperature -> 40 deg C

SUBSTAGE(2) 3 hours, 40 deg C

NTE regioselective

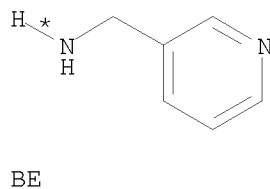
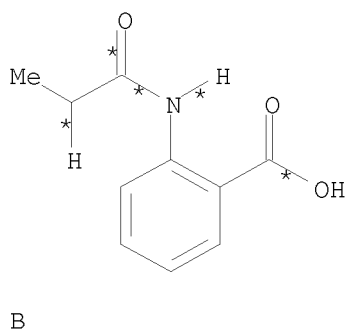
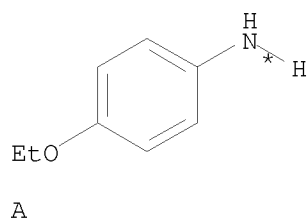
RX(6) RCT M 876016-38-5, R 108-00-9

PRO S 947535-98-0

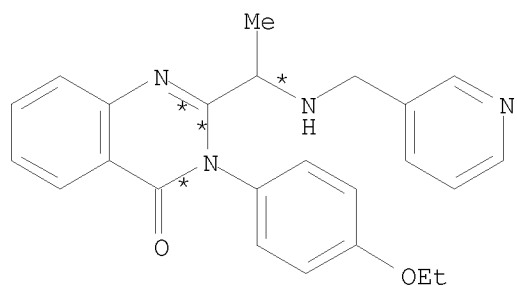
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SOL 64-17-5 EtOH  
CON 18 hours, reflux

RX(58) OF 112 COMPOSED OF RX(1), RX(4), RX(21)  
RX(58) A + B + BE ==> BF



3  
STEPS  
→



YIELD 40%

RX(1) RCT A 156-43-4, B 19165-26-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

CON room temperature

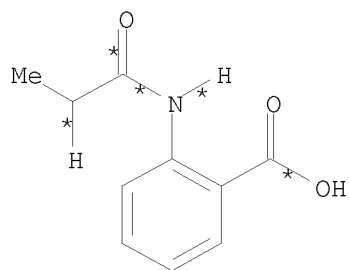
PRO C 93879-55-1

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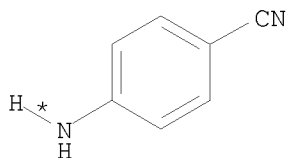
RX(4) RCT C 93879-55-1  
RGT N 127-09-3 AcONa, O 7726-95-6 Br2  
PRO M 876016-38-5  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature -> 40 deg C  
SUBSTAGE(2) 3 hours, 40 deg C  
NTE regioselective

RX(21) RCT BE 3731-52-0  
  
STAGE(1)  
RGT X 121-44-8 Et3N  
SOL 68-12-2 DMF  
CON 0.5 hours, room temperature  
  
STAGE(2)  
RCT M 876016-38-5  
CON overnight, room temperature  
  
PRO BF 947536-71-2

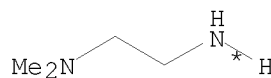
RX(61) OF 112 COMPOSED OF RX(2), RX(5), RX(7)  
RX(61) B + H + R ==> U



B



H



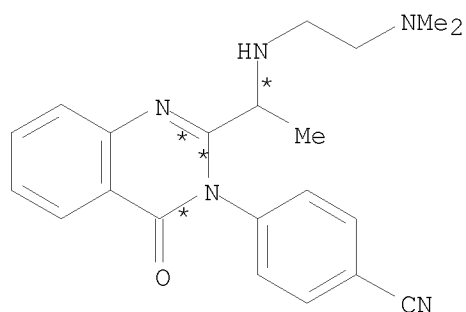
R

3

STEPS  
→



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U  
YIELD 47%

RX(2) RCT B 19165-26-5, H 873-74-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

CON room temperature

PRO I 860002-79-5

RX(5)

RCT I 860002-79-5

RGT N 127-09-3 AcONa, O 7726-95-6 Br2

PRO Q 860002-84-2

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) room temperature -> 40 deg C

SUBSTAGE(2) 3 hours, 40 deg C

NTE regioselective

RX(7)

RCT Q 860002-84-2, R 108-00-9

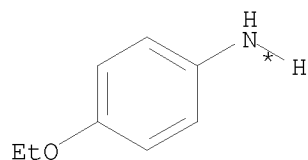
PRO U 860002-90-0

SOL 64-17-5 EtOH

CON 18 hours, reflux

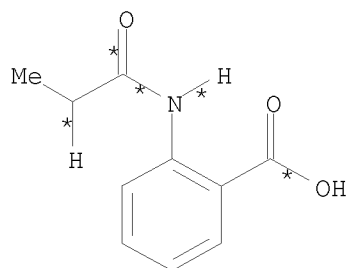
RX(67) OF 112 COMPOSED OF RX(1), RX(4), RX(6), RX(13)

RX(67) A + B + R + V ==> AK

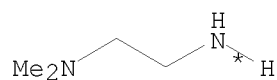


A

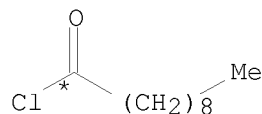
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B

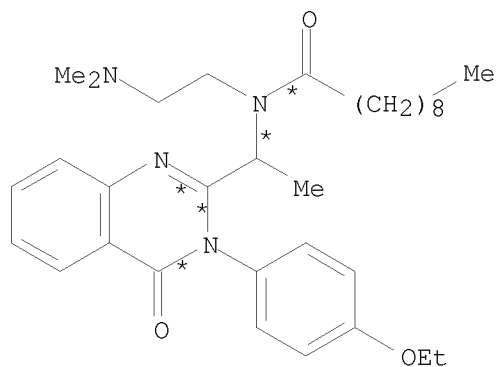


R



V

4  
STEPS  
→



AK  
YIELD 42%

RX(1) RCT A 156-43-4, B 19165-26-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

CON room temperature

PRO C 93879-55-1

RX(4) RCT C 93879-55-1

RGT N 127-09-3 AcONa, O 7726-95-6 Br2

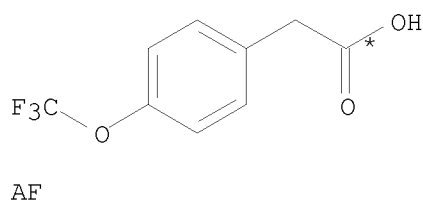
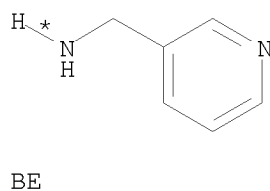
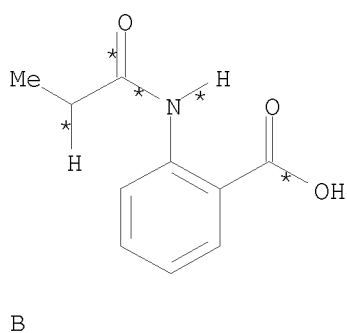
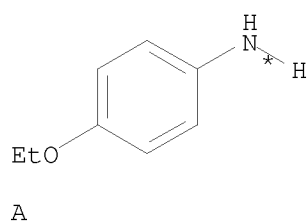
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PRO M 876016-38-5  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature -> 40 deg C  
SUBSTAGE(2) 3 hours, 40 deg C  
NTE regioselective

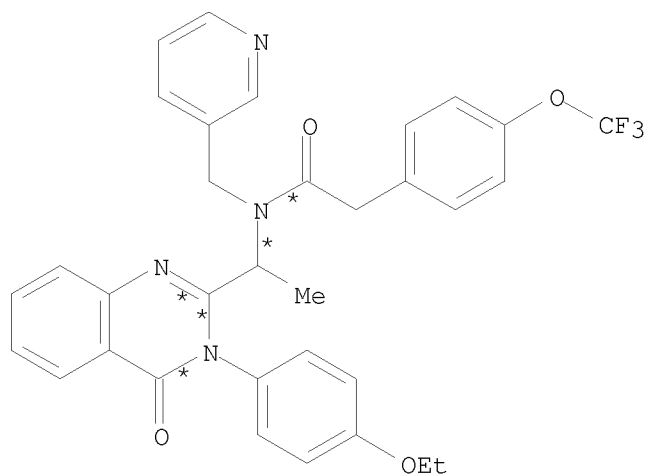
RX(6) RCT M 876016-38-5, R 108-00-9  
PRO S 947535-98-0  
SOL 64-17-5 EtOH  
CON 18 hours, reflux

RX(13) RCT V 112-13-0, S 947535-98-0  
RGT X 121-44-8 Et3N  
PRO AK 947536-01-8  
SOL 123-91-1 Dioxane  
CON 18 hours, room temperature

RX(68) OF 112 COMPOSED OF RX(1), RX(4), RX(21), RX(28)  
RX(68) A + B + BE + AF ==> BP



4  
STEPS  
→



BP  
YIELD 59%

RX(1) RCT A 156-43-4, B 19165-26-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na<sub>2</sub>CO<sub>3</sub>

SOL 7732-18-5 Water

CON room temperature

PRO C 93879-55-1

RX(4) RCT C 93879-55-1

RGT N 127-09-3 AcONa, O 7726-95-6 Br<sub>2</sub>

PRO M 876016-38-5

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) room temperature -> 40 deg C

SUBSTAGE(2) 3 hours, 40 deg C

NTE regioselective

RX(21) RCT BE 3731-52-0

STAGE(1)

RGT X 121-44-8 Et<sub>3</sub>N

SOL 68-12-2 DMF

CON 0.5 hours, room temperature

STAGE(2)

RCT M 876016-38-5

CON overnight, room temperature

PRO BF 947536-71-2

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RX(28) RCT AF 4315-07-5, BF 947536-71-2

STAGE(1)

RGT AH 25952-53-8 EDAP

CAT 68-12-2 DMF

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON overnight, room temperature

STAGE(2)

RGT AI 144-55-8 NaHCO<sub>3</sub>

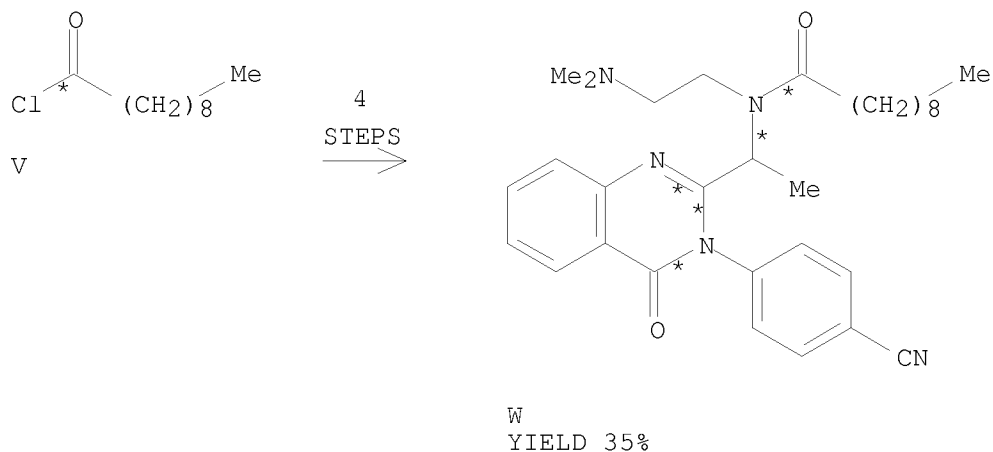
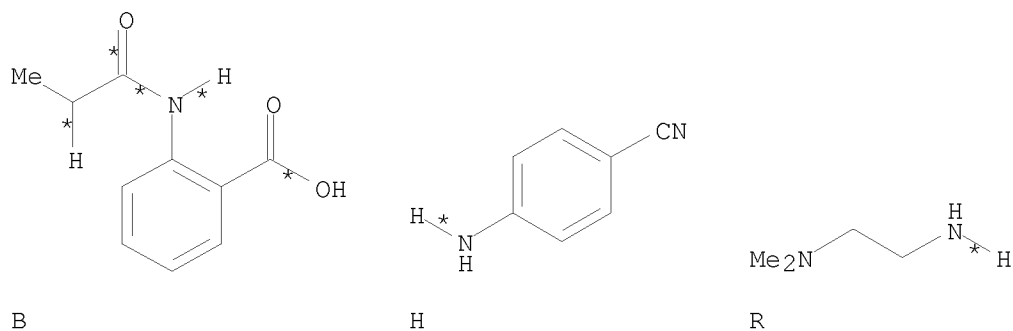
SOL 7732-18-5 Water

CON room temperature

PRO BP 473719-87-8

RX(74) OF 112 COMPOSED OF RX(2), RX(5), RX(7), RX(8)

RX(74) B + H + R + V ==> W



RX(2) RCT B 19165-26-5, H 873-74-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

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CON SUBSTAGE(1) room temperature -> reflux  
SUBSTAGE(2) 8 hours, reflux  
SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3  
SOL 7732-18-5 Water  
CON room temperature

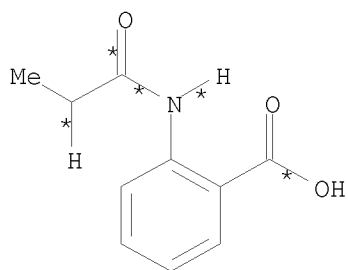
PRO I 860002-79-5

RX(5) RCT I 860002-79-5  
RGT N 127-09-3 AcONa, O 7726-95-6 Br2  
PRO Q 860002-84-2  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature -> 40 deg C  
SUBSTAGE(2) 3 hours, 40 deg C  
NTE regioselective

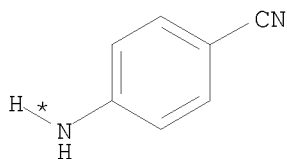
RX(7) RCT Q 860002-84-2, R 108-00-9  
PRO U 860002-90-0  
SOL 64-17-5 EtOH  
CON 18 hours, reflux

RX(8) RCT V 112-13-0, U 860002-90-0  
RGT X 121-44-8 Et3N  
PRO W 860002-95-5  
SOL 123-91-1 Dioxane  
CON 18 hours, room temperature

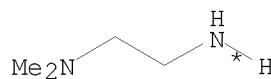
RX(75) OF 112 COMPOSED OF RX(2), RX(5), RX(7), RX(9)  
RX(75) B + H + R + Z ==> AA



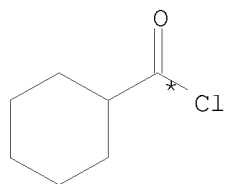
B



H



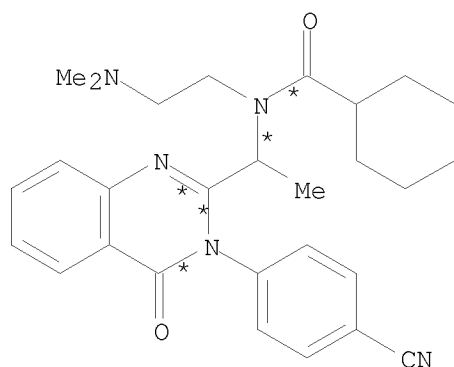
R



Z

4  
STEPS  
→

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AA  
YIELD 77%

RX(2) RCT B 19165-26-5, H 873-74-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na<sub>2</sub>CO<sub>3</sub>

SOL 7732-18-5 Water

CON room temperature

PRO I 860002-79-5

RX(5) RCT I 860002-79-5

RGT N 127-09-3 AcONa, O 7726-95-6 Br<sub>2</sub>

PRO Q 860002-84-2

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) room temperature -> 40 deg C

SUBSTAGE(2) 3 hours, 40 deg C

NTE regioselective

RX(7) RCT Q 860002-84-2, R 108-00-9

PRO U 860002-90-0

SOL 64-17-5 EtOH

CON 18 hours, reflux

RX(9) RCT Z 2719-27-9, U 860002-90-0

RGT X 121-44-8 Et<sub>3</sub>N

PRO AA 860003-01-6

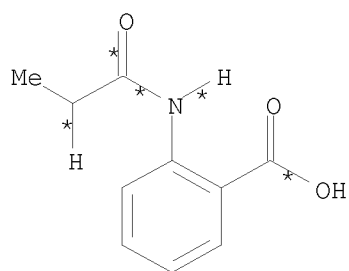
SOL 123-91-1 Dioxane

CON 18 hours, room temperature

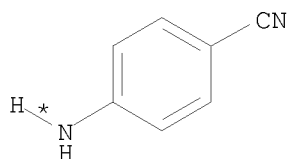
RX(76) OF 112 COMPOSED OF RX(2), RX(5), RX(7), RX(10)

RX(76) B + H + R + AB ==> AC

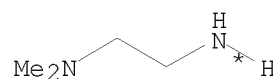
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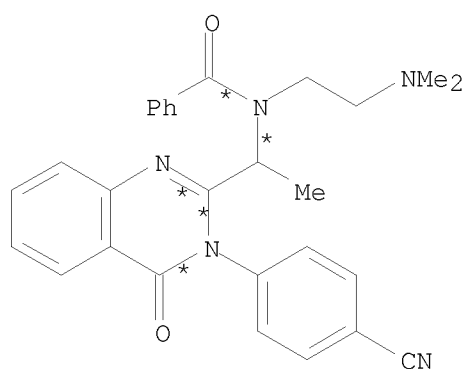
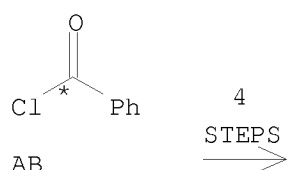
B



H



R



AC  
YIELD 22%

RX(2) RCT B 19165-26-5, H 873-74-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

CON room temperature

PRO I 860002-79-5

RX(5) RCT I 860002-79-5



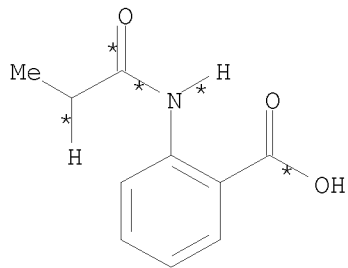
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RGT N 127-09-3 AcONa, O 7726-95-6 Br2  
PRO Q 860002-84-2  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature -> 40 deg C  
SUBSTAGE(2) 3 hours, 40 deg C  
NTE regioselective

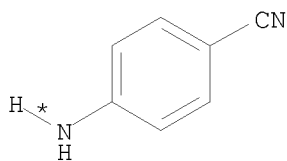
RX(7) RCT Q 860002-84-2, R 108-00-9  
PRO U 860002-90-0  
SOL 64-17-5 EtOH  
CON 18 hours, reflux

RX(10) RCT AB 98-88-4, U 860002-90-0  
RGT X 121-44-8 Et3N  
PRO AC 860003-03-8  
SOL 123-91-1 Dioxane  
CON 18 hours, room temperature

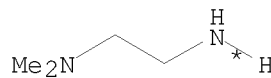
RX(77) OF 112 COMPOSED OF RX(2), RX(5), RX(7), RX(11)  
RX(77) B + H + R + AD ==> AE



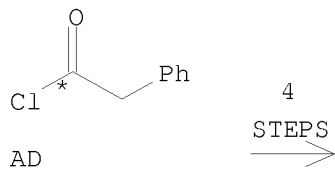
B



H

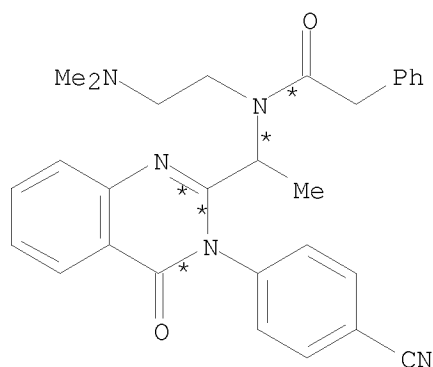


R



AD

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AE  
YIELD 40%

RX(2) RCT B 19165-26-5, H 873-74-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na<sub>2</sub>CO<sub>3</sub>

SOL 7732-18-5 Water

CON room temperature

PRO I 860002-79-5

RX(5)

RCT I 860002-79-5

RGT N 127-09-3 AcONa, O 7726-95-6 Br<sub>2</sub>

PRO Q 860002-84-2

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) room temperature -> 40 deg C

SUBSTAGE(2) 3 hours, 40 deg C

NTE regioselective

RX(7)

RCT Q 860002-84-2, R 108-00-9

PRO U 860002-90-0

SOL 64-17-5 EtOH

CON 18 hours, reflux

RX(11)

RCT AD 103-80-0, U 860002-90-0

RGT X 121-44-8 Et<sub>3</sub>N

PRO AE 947535-99-1

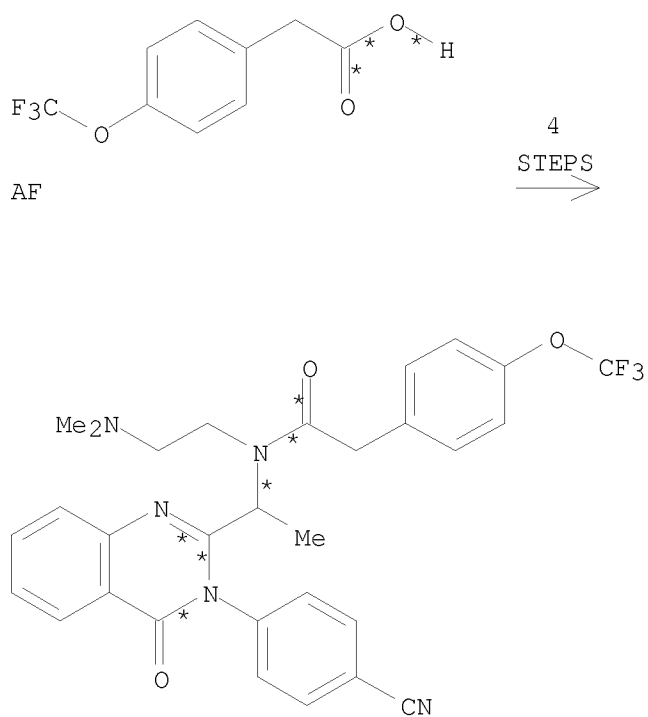
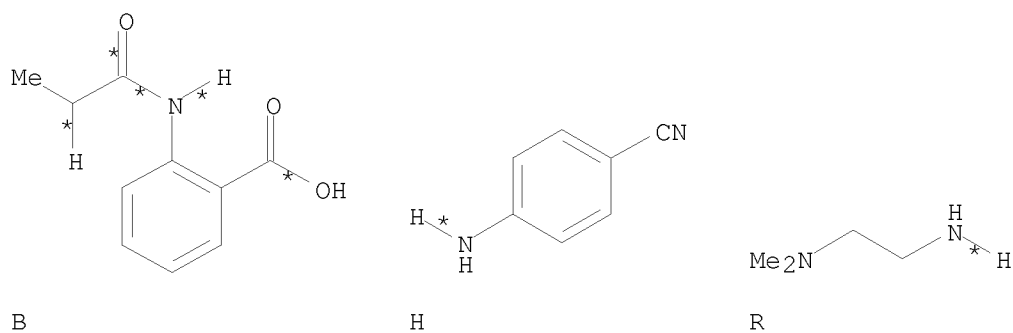
SOL 123-91-1 Dioxane

CON 18 hours, room temperature

RX(78) OF 112 COMPOSED OF RX(2), RX(5), RX(7), RX(12)

RX(78) B + H + R + AF ==> AG

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AG  
YIELD 47%

RX(2) RCT B 19165-26-5, H 873-74-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

CON room temperature

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PRO I 860002-79-5

RX(5) RCT I 860002-79-5  
RGT N 127-09-3 AcONa, O 7726-95-6 Br2  
PRO Q 860002-84-2  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature -> 40 deg C  
SUBSTAGE(2) 3 hours, 40 deg C  
NTE regioselective

RX(7) RCT Q 860002-84-2, R 108-00-9  
PRO U 860002-90-0  
SOL 64-17-5 EtOH  
CON 18 hours, reflux

RX(12) RCT AF 4315-07-5, U 860002-90-0

STAGE(1)  
RGT AH 25952-53-8 EDAP  
CAT 68-12-2 DMF  
SOL 75-09-2 CH2Cl2  
CON overnight, room temperature

STAGE(2)  
RGT AI 144-55-8 NaHCO3  
SOL 7732-18-5 Water  
CON room temperature

PRO AG 947536-00-7

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 15 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 147:301069 CASREACT

TITLE: Synthesis and behavior of  
2-carboxyvinyl-6,8-dibromo-4H-3,1-benzoxazin-4-one  
towards nitrogen, carbon, and sulfur nucleophiles

AUTHOR(S): Abdel-Rahman, T. M.; El-Hashash, M. A.; El-Badry, Y.  
A.

CORPORATE SOURCE: Faculty of Specific Education, Ain Shams University,  
Cairo, Egypt

SOURCE: Egyptian Journal of Chemistry (2005), 48(6), 679-693  
CODEN: EGJCA3; ISSN: 0449-2285

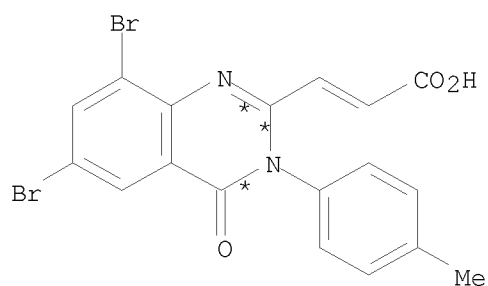
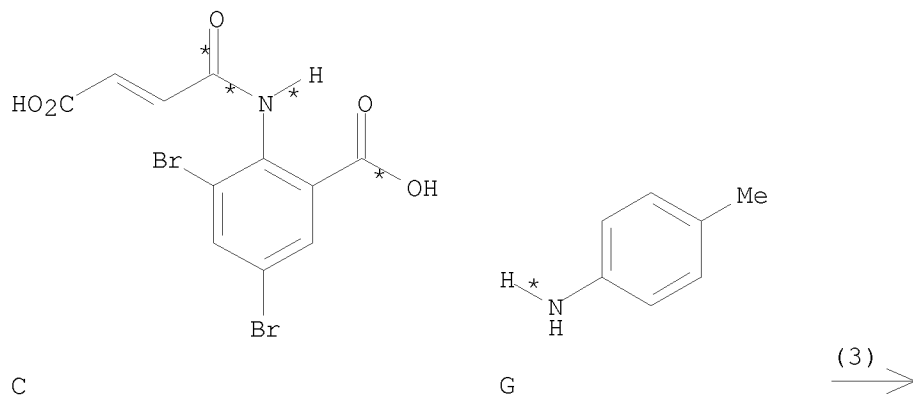
PUBLISHER: National Information and Documentation Centre

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 3-(6,8-Dibromo-4-oxo-4H-benzo[d][1,3]oxazin-2-yl)acrylic acid (I) was synthesized and allowed to react with some nitrogen nucleophiles to afford 3-substituted quinazolinones and benzamide derivs. 3-(6,8-Dibromo-3-hydroxy-4-oxo-3,4-dihydroquinazolin-2-yl)acrylic acid was subjected to acylation and alkylation. Also, 3-(6,8-dibromo-3-(2-hydroxyethyl)-4-oxo-3,4-dihydroquinazolin-2-yl)acrylic acid was used to alkylate some aromatic systems. Treatment of I with o-phenylenediamine in different solvents under different conditions furnished a substituted benzamide and 3-substituted quinazolinone. I was converted to 4(3H)-quinazolinone by treatment with formamide and/or

ammonium acetate which was alkylated with Et chloroacetate and treated with hydrazine hydrate to produced the hydrazide. Interaction of I with hydrazine hydrate gave an unexpected fused quinazolinone, which was confirmed by its interaction with acid chlorides. Oxazinone ring cleavage occurred by the use of active methylene containing compds. under different conditions.

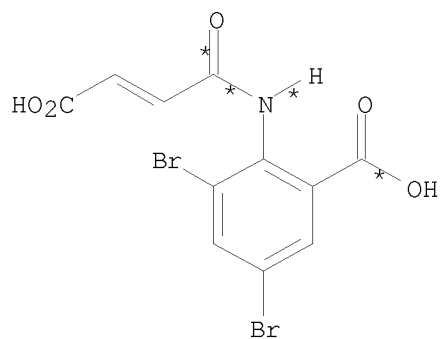
$$RX(3) \text{ OF } 64 \dots C + G \implies H$$


YIELD 48%

RX(3) RCT C 934242-55-4, G 106-49-0  
RGT I 64-19-7 AcOH  
PRO H 934242-56-5  
SOL 64-19-7 AcOH  
CON SUBSTAGE(1) 3 hours, reflux  
SUBSTAGE(2) cooled

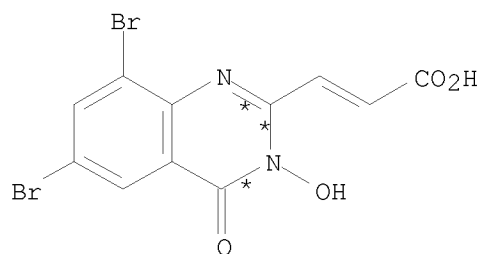
RX (4) OF 64                    ...C        ==> J...

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C

(4)  $\longrightarrow$

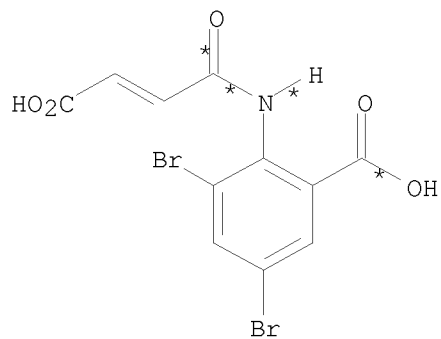


J

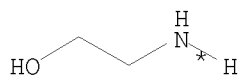
YIELD 73%

RX(4)      RCT   C 934242-55-4  
 RGT   K 5470-11-1 H2NOH-HCl  
 PRO   J 934242-57-6  
 SOL   110-86-1 Pyridine  
 CON   SUBSTAGE(1) 3 hours, reflux  
       SUBSTAGE(2) cooled

RX(5) OF 64      ...C + M ==> N...



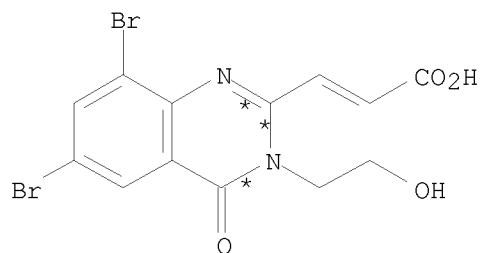
C



M

(5)  $\longrightarrow$

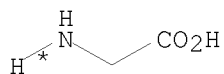
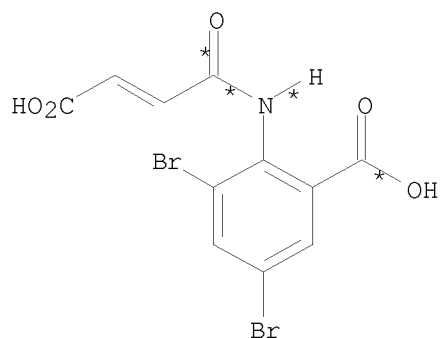
10/ 562,112



N  
YIELD 58%

RX(5)      RCT    C 934242-55-4, M 141-43-5  
               RGT    O 127-09-3 AcONa  
               PRO    N 934242-58-7  
               SOL    64-19-7 AcOH  
               CON    SUBSTAGE(1) 3 hours, reflux  
                      SUBSTAGE(2) cooled

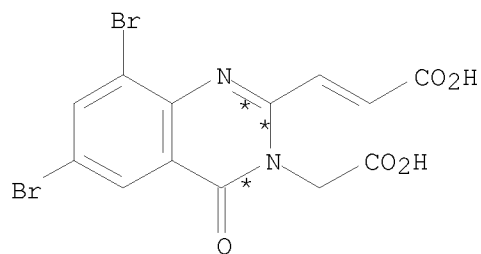
RX(6) OF 64      ...C + P ==> Q



C

P

(6)  $\longrightarrow$



Q  
YIELD 44%

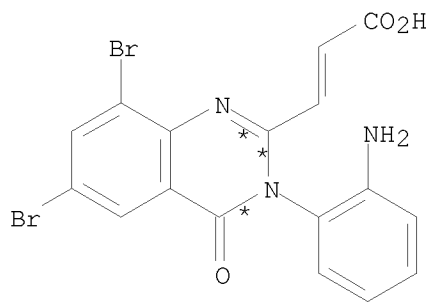
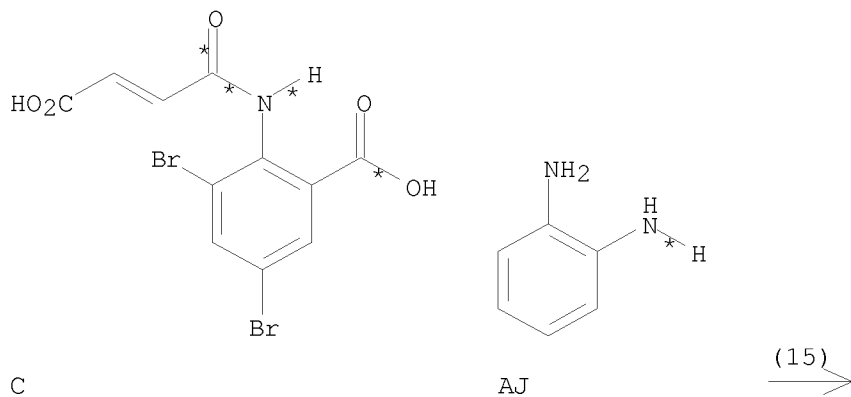
10/ 562,112

```

RX(6)      RCT  C 934242-55-4, P 56-40-6
           RGT  L 110-86-1 Pyridine
           PRO  Q 934242-59-8
           SOL  110-86-1 Pyridine
           CON  SUBSTAGE(1) 8 hours, reflux
                SUBSTAGE(2) cooled

```

RX(15) OF 64 ...C + AJ ==> AL



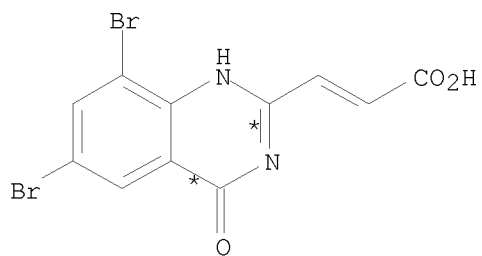
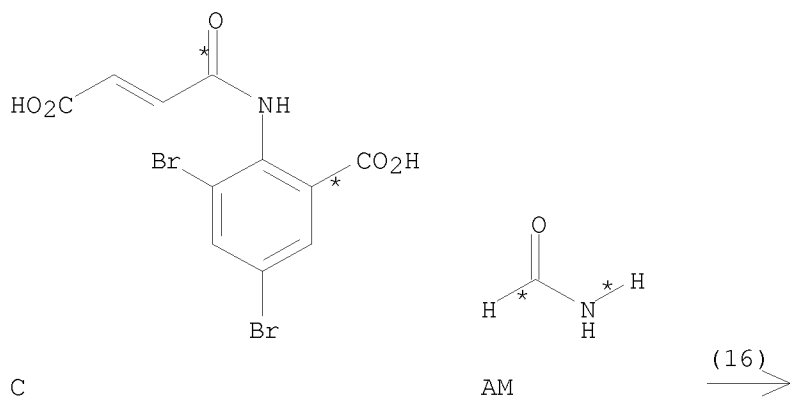
AL  
YIELD 56%

RX(15)	RCT	C 934242-55-4, AJ 95-54-5
	RGT	O 127-09-3 AcONa
	PRO	AL 934242-68-9
	SOL	64-19-7 AcOH
	CON	SUBSTAGE(1) 2 hours, reflux
		SUBSTAGE(2) cooled
	NTE	product depends on reaction conditions

RX(16) OF 64 ...C + AM ==> AN...

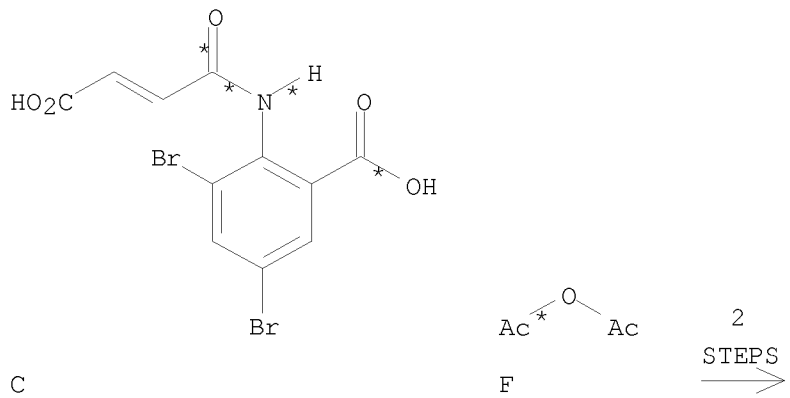


10/ 562,112

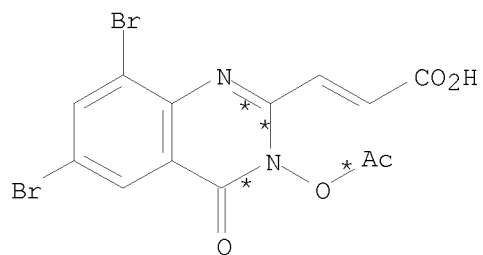


AN  
YIELD 65%

RX(16) RCT C 934242-55-4, AM 75-12-7  
PRO AN 934242-69-0  
SOL 75-12-7 Formamide  
CON SUBSTAGE(1) 2 hours, reflux  
SUBSTAGE(2) cooled

$$\begin{array}{l} \text{RX(44) OF 64 COMPOSED OF RX(4), RX(9)} \\ \text{RX(44) C + F ==> W} \end{array}$$


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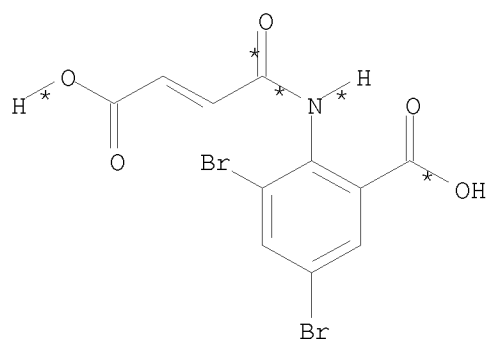


W  
YIELD 80%

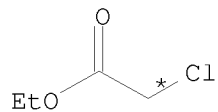
RX(4)      RCT    C 934242-55-4  
             RGT    K 5470-11-1 H2NOH-HCl  
             PRO    J 934242-57-6  
             SOL    110-86-1 Pyridine  
             CON    SUBSTAGE(1) 3 hours, reflux  
                     SUBSTAGE(2) cooled

RX(9)      RCT    J 934242-57-6, F 108-24-7  
             PRO    W 934242-62-3  
             SOL    108-24-7 Ac2O  
             CON    SUBSTAGE(1) 2 hours, reflux  
                     SUBSTAGE(2) cooled

RX(45) OF 64 COMPOSED OF RX(4), RX(10)  
RX(45)      C    +    2 X    ==>    Y



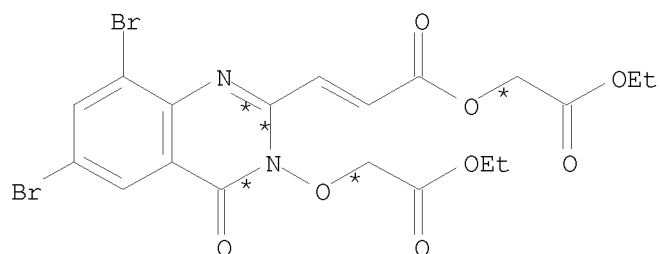
C



2 X

2  
STEPS  
→

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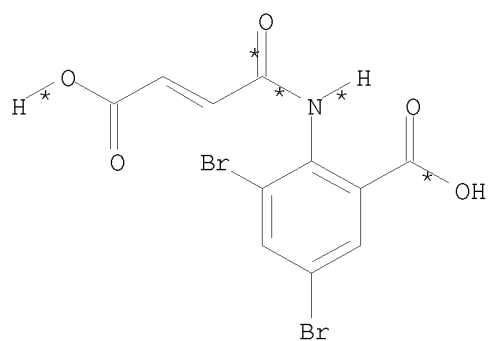


Y  
YIELD 28%

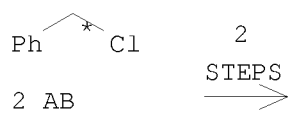
RX(4)      RCT    C 934242-55-4  
              RGT    K 5470-11-1 H2NOH-HCl  
              PRO    J 934242-57-6  
              SOL    110-86-1 Pyridine  
              CON    SUBSTAGE(1) 3 hours, reflux  
                      SUBSTAGE(2) cooled

RX(10)     RCT    J 934242-57-6, X 105-39-5  
              RGT    Z 584-08-7 K2CO3  
              PRO    Y 934242-63-4  
              SOL    67-64-1 Me2CO  
              CON    24 hours, reflux

RX(46) OF 64 COMPOSED OF RX(4), RX(11)  
 RX(46)      C    +    2 AB    ==>    AC

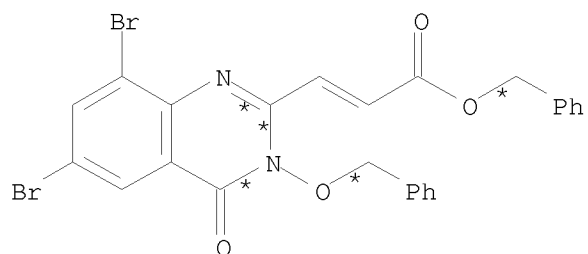


C



2  
STEPS  
→

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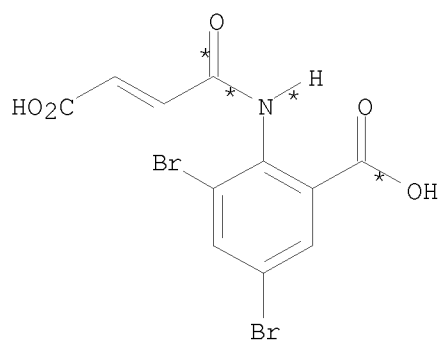


AC  
YIELD 37%

RX(4)      RCT    C 934242-55-4  
             RGT    K 5470-11-1 H2NOH-HCl  
             PRO    J 934242-57-6  
             SOL    110-86-1 Pyridine  
             CON    SUBSTAGE(1) 3 hours, reflux  
                     SUBSTAGE(2) cooled

RX(11)     RCT    J 934242-57-6, AB 100-44-7  
             RGT    Z 584-08-7 K2CO3  
             PRO    AC 934242-64-5  
             SOL    67-64-1 Me2CO  
             CON    24 hours, reflux

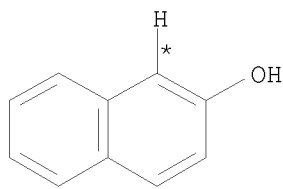
RX(47) OF 64 COMPOSED OF RX(5), RX(12)  
RX(47)      C + M + AD ==> AE



C



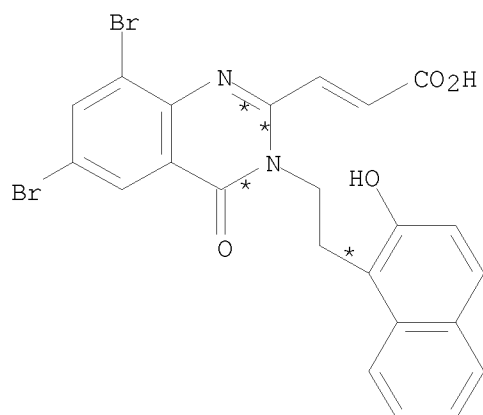
M



AD

2  
STEPS  
→

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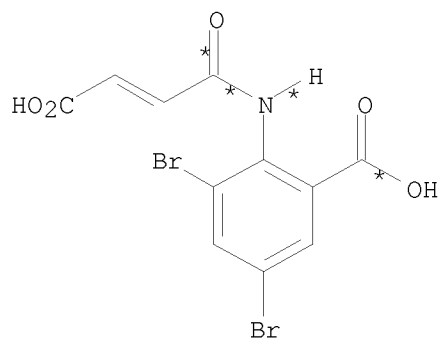


AE  
YIELD 38%

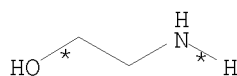
RX(5)      RCT    C 934242-55-4, M 141-43-5  
              RGT    O 127-09-3 AcONa  
              PRO    N 934242-58-7  
              SOL    64-19-7 AcOH  
              CON    SUBSTAGE(1) 3 hours, reflux  
                      SUBSTAGE(2) cooled

RX(12)     RCT    N 934242-58-7, AD 135-19-3  
              PRO    AE 934242-65-6  
              CAT    7647-01-0 HCl  
              SOL    7732-18-5 Water, 64-17-5 EtOH  
              CON    SUBSTAGE(1) 6 hours, heated  
                      SUBSTAGE(2) cooled

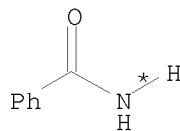
RX(48) OF 64 COMPOSED OF RX(5), RX(13)  
 RX(48)      C    +    M    +    AH    ==>    AI



C



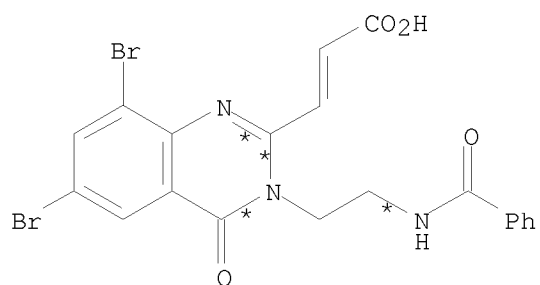
M



AH

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2  
STEPS  
→

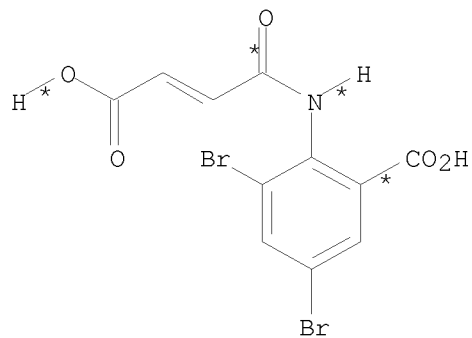


AI  
YIELD 44%

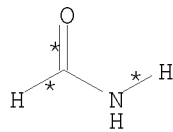
RX(5)      RCT    C 934242-55-4, M 141-43-5  
             RGT    O 127-09-3 AcONa  
             PRO    N 934242-58-7  
             SOL    64-19-7 AcOH  
             CON    SUBSTAGE(1) 3 hours, reflux  
                     SUBSTAGE(2) cooled

RX(13)     RCT    N 934242-58-7, AH 55-21-0  
             PRO    AI 934242-66-7  
             CAT    7647-01-0 HCl  
             SOL    7732-18-5 Water, 64-17-5 EtOH  
             CON    SUBSTAGE(1) 6 hours, heated  
                     SUBSTAGE(2) cooled

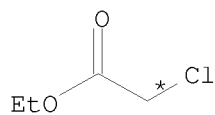
RX(49) OF 64 COMPOSED OF RX(16), RX(17)  
RX(49)      C + AM + 2 X ==> AO



C



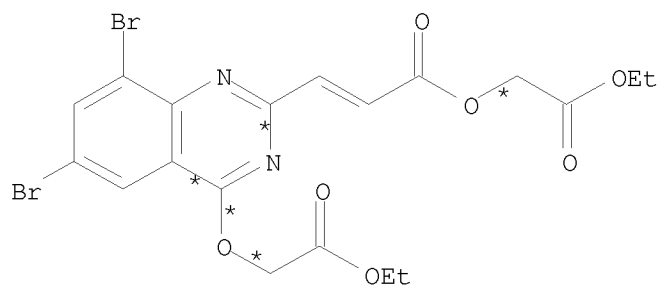
AM



2 X

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2  
STEPS  
→

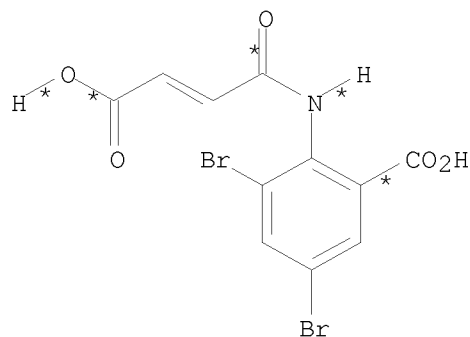


AO  
YIELD 32%

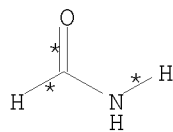
RX(16) RCT C 934242-55-4, AM 75-12-7  
PRO AN 934242-69-0  
SOL 75-12-7 Formamide  
CON SUBSTAGE(1) 2 hours, reflux  
SUBSTAGE(2) cooled

RX(17) RCT X 105-39-5, AN 934242-69-0  
RGT Z 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO AO 934242-70-3  
SOL 67-64-1 Me<sub>2</sub>CO  
CON 25 hours, reflux

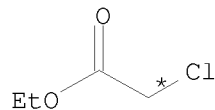
RX(63) OF 64 COMPOSED OF RX(16), RX(17), RX(18)  
RX(63) C + AM + 2 X ==> AP



C

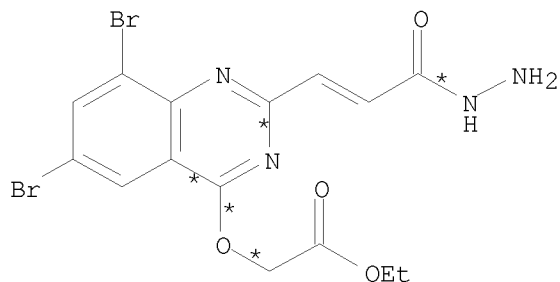


AM



2 X

3  
STEPS  
→



AP  
YIELD 57%

RX(16) RCT C 934242-55-4, AM 75-12-7  
PRO AN 934242-69-0  
SOL 75-12-7 Formamide  
CON SUBSTAGE(1) 2 hours, reflux  
SUBSTAGE(2) cooled

RX(17) RCT X 105-39-5, AN 934242-69-0  
RGT Z 584-08-7 K2CO3  
PRO AO 934242-70-3  
SOL 67-64-1 Me2CO  
CON 25 hours, reflux

RX(18) RCT AO 934242-70-3  
RGT AQ 7803-57-8 N2H4-H2O  
PRO AP 934242-71-4  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 6 hours, reflux  
SUBSTAGE(2) cooled

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 16 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 147:277558 CASREACT

TITLE: Synthesis, characterization, chelating properties and  
anti-fungal activity of  
2-(4-phenylpiperazinyl)methyl-3-(8-quinolinol-5-yl)-  
4(3H)-quinazolinone

AUTHOR(S): Shelat, C. D.; Vashi, R. T.

CORPORATE SOURCE: Department of Chemistry, Navyug Science College,  
Surat, 395 000, India

SOURCE: E-Journal of Chemistry (2005), 2(6), 86-90

CODEN: ECJHAO

URL: <http://cc.lasphost.com/namfarook/NEWEJC/VOL2/SIXTH/fulltext/86-90.pdf>

PUBLISHER: WWW Publications

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

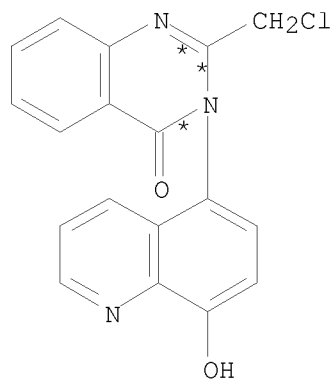
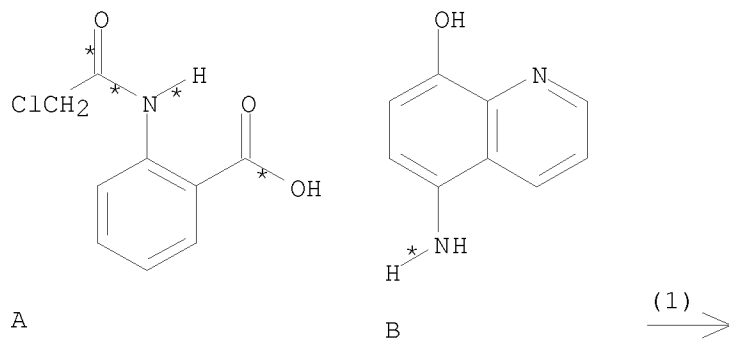
AB Title compds. were prepared from 2-HO2CC6H4NHC(=O)CH2Cl, 5-amino-8-quinolinol,



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and N-phenylpiperazine and characterized. Various transition metal (Cu<sup>2+</sup>, Co<sup>2+</sup>, Ni<sup>2+</sup>, Zn<sup>2+</sup>, Mn<sup>2+</sup>) chelates were prepared and characterized by metal ligand (M:L) ratio, IR and reflectance spectral studies, magnetic moment, and antimicrobial activity.

RX(1) OF 18      A + B ==> C...



C

RX(1)      RCT   A 14422-49-2, B 13207-66-4

STAGE(1)

RGT   D 7719-12-2 PC13

SOL   108-88-3 PhMe

CON   9 hours, reflux

STAGE(2)

RGT   E 7732-18-5 Water

CON   cooled

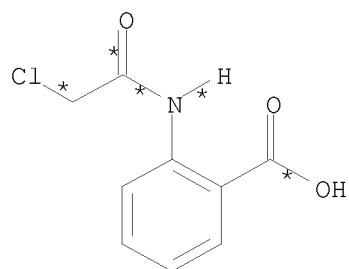
PRO   C 946052-78-4

NTE   regioselective

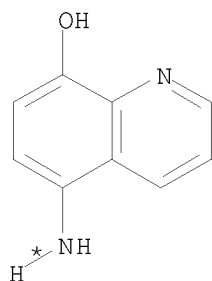
RX(8) OF 18 COMPOSED OF RX(1), RX(2)

RX(8)      A + B + G ==> H

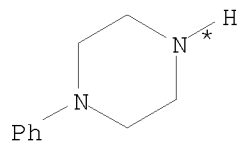
10/ 562,112



A

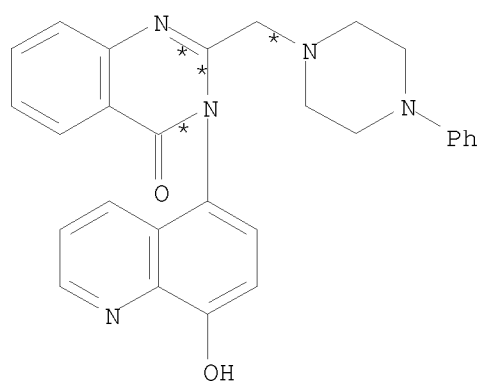


B



G

2  
STEPS  
→



H

YIELD 80%

RX(1) RCT A 14422-49-2, B 13207-66-4

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 9 hours, reflux

STAGE(2)

RGT E 7732-18-5 Water

CON cooled

PRO C 946052-78-4

NTE regioselective

RX(2) RCT C 946052-78-4, G 92-54-6

PRO H 946052-79-5

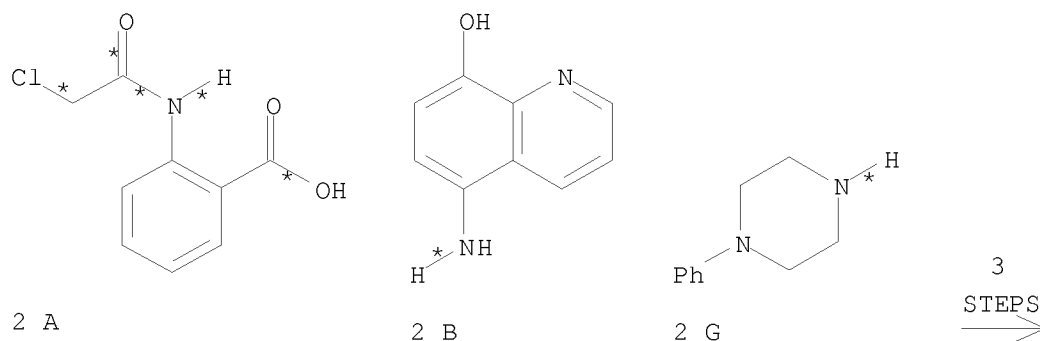
SOL 110-86-1 Pyridine

CON 10 hours, reflux

RX(14) OF 18 COMPOSED OF RX(1), RX(2), RX(3)

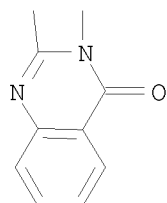
RX(14) 2 A + 2 B + 2 G ==> J

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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 2-A



J  
YIELD 83%

RX(1) RCT A 14422-49-2, B 13207-66-4

STAGE(1)

RGT D 7719-12-2 PC13  
SOL 108-88-3 PhMe  
CON 9 hours, reflux

STAGE(2)

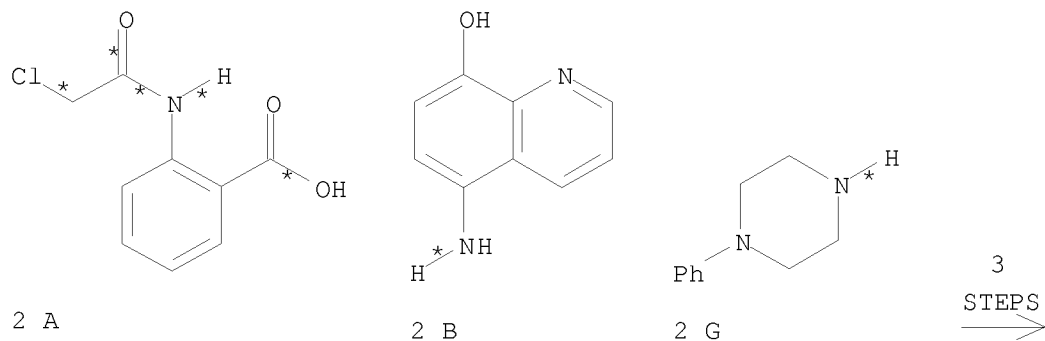
RGT E 7732-18-5 Water  
CON cooled

PRO C 946052-78-4  
NTE regioselective

RX(2) RCT C 946052-78-4, G 92-54-6  
PRO H 946052-79-5  
SOL 110-86-1 Pyridine  
CON 10 hours, reflux

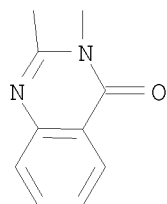
RX(3) RCT H 946052-79-5  
RGT K 127-09-3 AcONa, L 64-18-6 HCO<sub>2</sub>H, M 142-71-2 Cu(OAc)<sub>2</sub>  
PRO J 946052-80-8  
SOL 7732-18-5 Water  
CON 2 hours, heated

RX(15) OF 18 COMPOSED OF RX(1), RX(2), RX(4)

$$\text{RX(15)} \quad 2 \text{ A} + 2 \text{ B} + 2 \text{ G} \implies \text{N}$$


\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 2-A



N  
YIELD 89%

RX(1) RCT A 14422-49-2, B 13207-66-4

STAGE (1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 9 hours, reflux

STAGE (2)

RGT E 7732-18-5 Water

CON      cooled

PRO C 946052-78-4

NTE regioselective

RX(2) RCT C 946052-78-4, G 92-54-6

PRO H 946052-79-5

SOL 110-86-1 Pyridine

CON 10 hours, reflux

RX (4) RCT H 946052-79-5

RGT O 71-48-7  $\text{Co}(\text{OAc})_2$ , K 127-09-3  $\text{AcONa}$ , L 64-18-6  $\text{HCO}_2\text{H}$

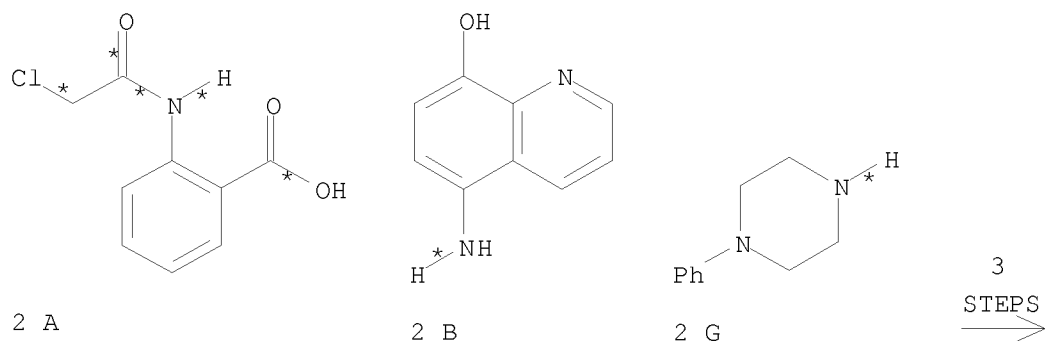
PRO N 946052-81-9

SOL 7732-18-5 Water

CON 2 hours, heated

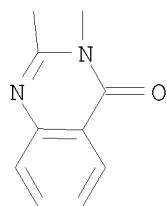
10/ 562,112

RX(16) OF 18 COMPOSED OF RX(1), RX(2), RX(5)  
RX(16) 2 A + 2 B + 2 G ==> P



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 2-A



P  
YIELD 79%

RX(1) RCT A 14422-49-2, B 13207-66-4

STAGE(1)

RGT D 7719-12-2 PC13  
SOL 108-88-3 PhMe  
CON 9 hours, reflux

STAGE(2)

RGT E 7732-18-5 Water  
CON cooled

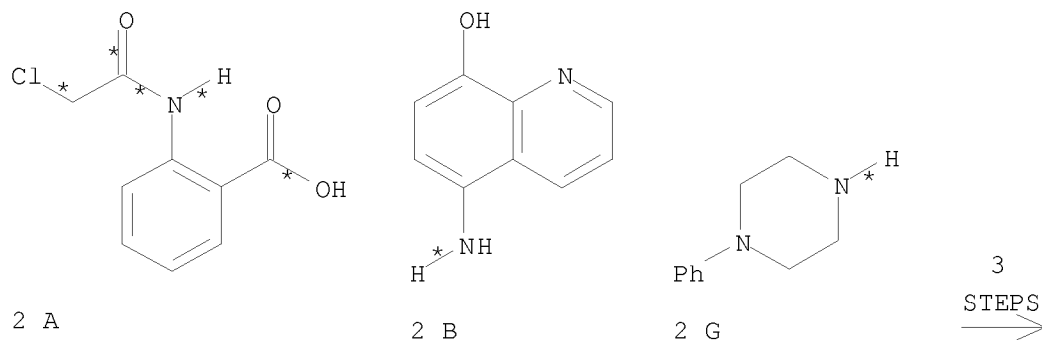
PRO C 946052-78-4  
NTE regioselective

RX(2) RCT C 946052-78-4, G 92-54-6  
PRO H 946052-79-5  
SOL 110-86-1 Pyridine  
CON 10 hours, reflux

RX(5) RCT H 946052-79-5  
RGT Q 373-02-4 Ni(OAc)<sub>2</sub>, K 127-09-3 AcONa, L 64-18-6 HCO<sub>2</sub>H  
PRO P 946052-82-0  
SOL 7732-18-5 Water  
CON 2 hours, heated

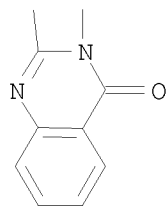
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RX(17) OF 18 COMPOSED OF RX(1), RX(2), RX(6)  
RX(17) 2 A + 2 B + 2 G ==> R



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 2-A



R  
YIELD 86%

RX(1) RCT A 14422-49-2, B 13207-66-4

STAGE(1)

RGT D 7719-12-2 PC13  
SOL 108-88-3 PhMe  
CON 9 hours, reflux

STAGE(2)

RGT E 7732-18-5 Water  
CON cooled

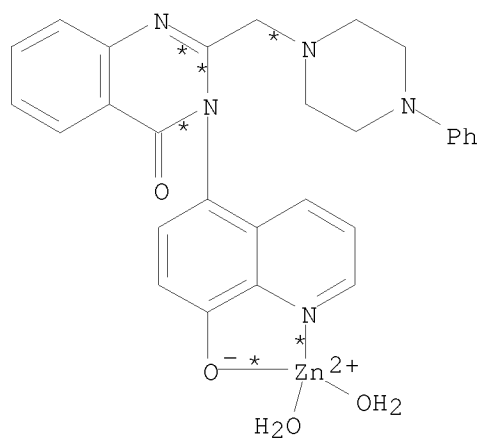
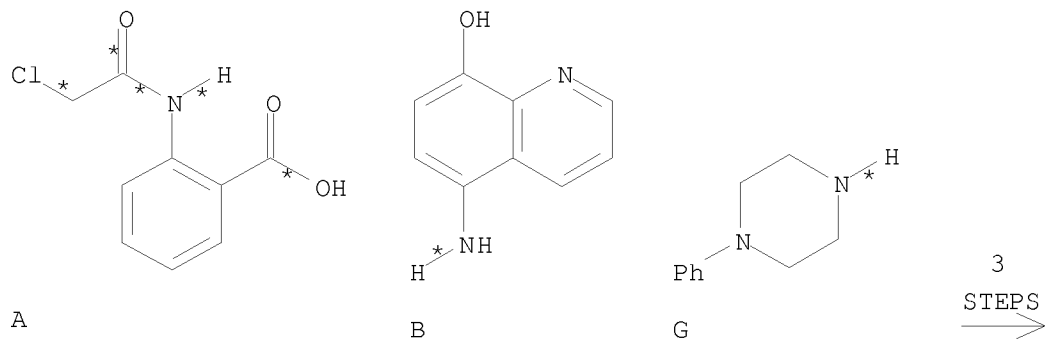
PRO C 946052-78-4  
NTE regioselective

RX(2) RCT C 946052-78-4, G 92-54-6  
PRO H 946052-79-5  
SOL 110-86-1 Pyridine  
CON 10 hours, reflux

RX(6) RCT H 946052-79-5  
RGT S 638-38-0 Mn(OAc)2, K 127-09-3 AcONa, L 64-18-6 HCO2H  
PRO R 946052-83-1  
SOL 7732-18-5 Water  
CON 2 hours, heated

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RX(18) OF 18 COMPOSED OF RX(1), RX(2), RX(7)  
RX(18) A + B + G ==> T



T  
YIELD 88%

RX(1) RCT A 14422-49-2, B 13207-66-4

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 9 hours, reflux

STAGE(2)

RGT E 7732-18-5 Water

CON cooled

PRO C 946052-78-4

NTE regioselective

RX(2) RCT C 946052-78-4, G 92-54-6

PRO H 946052-79-5

SOL 110-86-1 Pyridine

CON 10 hours, reflux

RX(7)       RCT   H 946052-79-5  
              RGT   U 557-34-6 Zn(OAc)<sub>2</sub>, K 127-09-3 AcONa, L 64-18-6 HCO<sub>2</sub>H  
              PRO   T 946052-84-2  
              SOL   7732-18-5 Water  
              CON   2 hours, heated

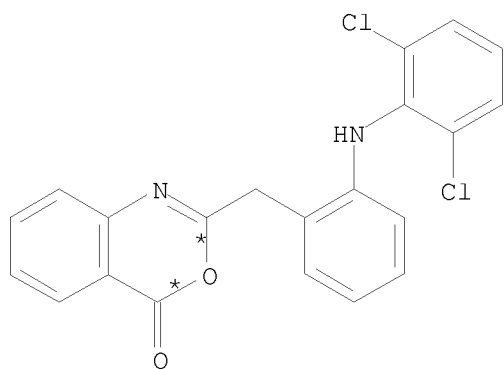
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L3 ANSWER 17 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 147:235107 CASREACT
TITLE: Quinazolin-4(3H)-ones of
2-[(2',6'-dichlorophenyl)amino]phenyl acetic acid with
substituted aryl acetamide and their microbial studies
AUTHOR(S): Patel, N. B.; Chaudhari, R. C.
CORPORATE SOURCE: Department of Chemistry, Veer Narmad South Gujarat
University, Surat, 395 007, India
SOURCE: Journal of the Indian Chemical Society (2006), 83(8),
838-841
CODEN: JICSAH; ISSN: 0019-4522
PUBLISHER: Indian Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI
```

AB Synthesis and antimicrobial activity of quinazolinones I (X = 1,4-C<sub>6</sub>H<sub>4</sub>, bond; R = H, 2-NO<sub>2</sub>, 3-NO<sub>2</sub>, 4-NO<sub>2</sub>, 2-Me, 3-Me, 4-Me, 2-MeO, 4-MeO, 2-Cl, 3-Cl, 4-Cl; R<sub>1</sub> = H, Br) were reported from [(2,6-dichlorophenyl)amino]phenylacetic acid and appropriate N-arylacetamides via benzoxazine II (R = H, Br). All the compds. were established on the basis of spectral data (IR, <sup>1</sup>H NMR) and elemental anal.

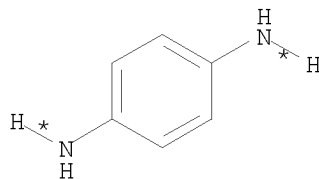
RX(1) OF 48            A + B + C ==> D



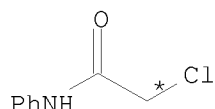
10/ 562,112



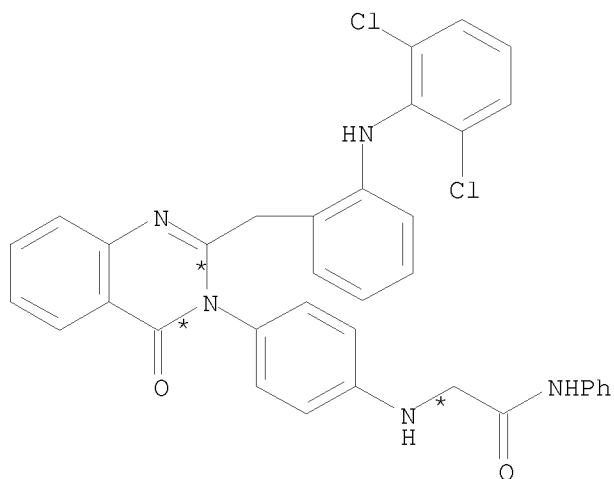
A



B



C



D  
YIELD 31%

RX(1) RCT A 402950-18-9, B 106-50-3

STAGE(1)

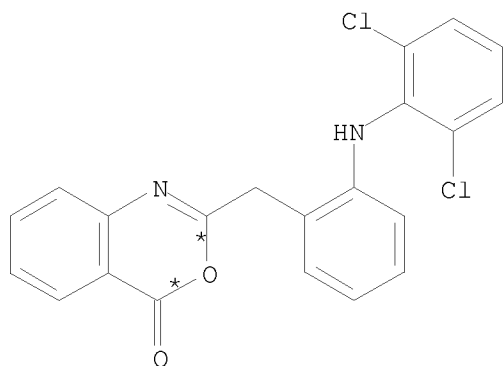
SOL 110-86-1 Pyridine  
CON reflux

STAGE(2)

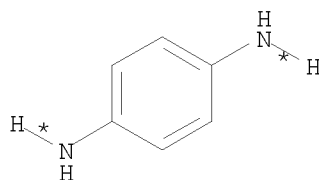
RCT C 587-65-5  
SOL 67-56-1 MeOH  
CON reflux

PRO D 945486-73-7

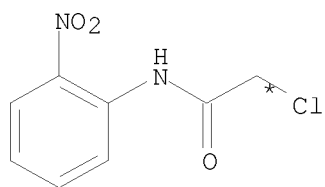
RX(2) OF 48 A + B + G ==> H



A



B



G



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT A 402950-18-9, B 106-50-3

STAGE(1)

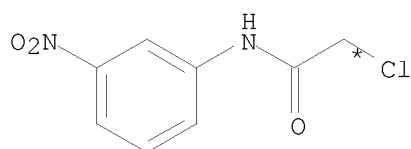
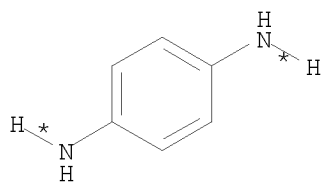
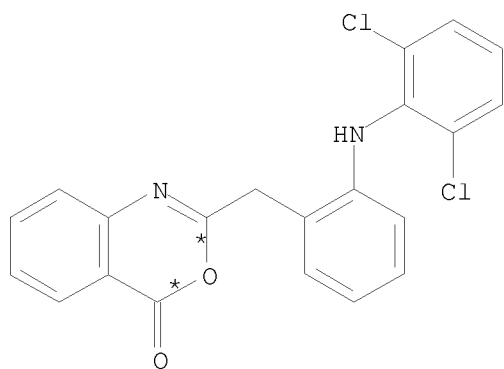
SOL 110-86-1 Pyridine  
CON reflux

STAGE(2)

RCT G 10147-70-3  
SOL 67-56-1 MeOH  
CON reflux

PRO H 945486-74-8

RX(3) OF 48 A + B + I ==> J



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(3) RCT A 402950-18-9, B 106-50-3

STAGE (1)

SOL 110-86-1 Pyridine

CON reflux

STAGE (2)

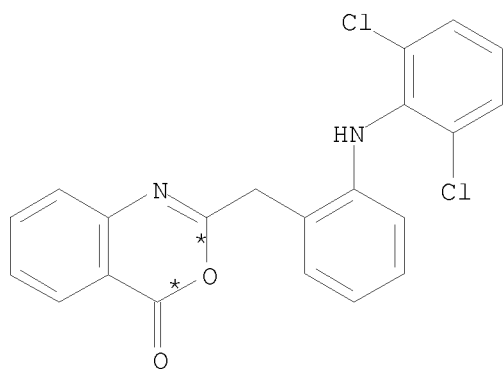
RCT I 10147-71-4

SOL 67-56-1 MeOH

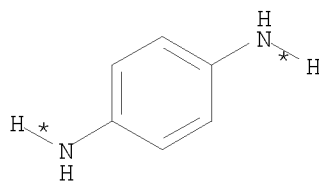
CON reflux

PRO J 945486-75-9

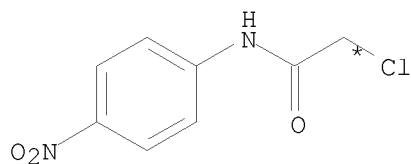
RX (4) OF 48            A + B + K ==> L



A



B



K



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(4) RCT A 402950-18-9, B 106-50-3

STAGE(1)

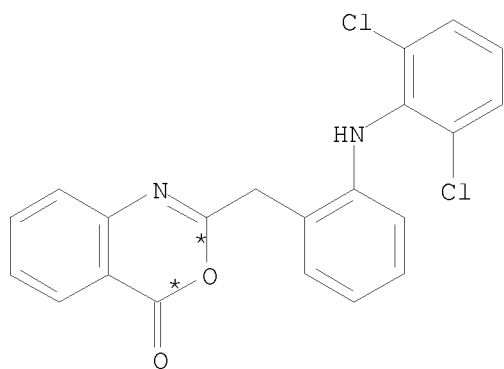
SOL 110-86-1 Pyridine  
CON reflux

STAGE(2)

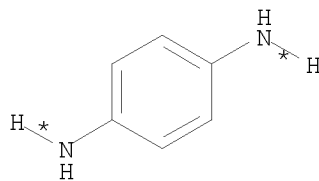
RCT K 17329-87-2  
SOL 67-56-1 MeOH  
CON reflux

PRO L 945486-76-0

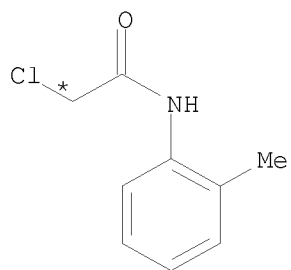
RX(5) OF 48 A + B + M ==> N



A



B



M

(5)  $\longrightarrow$ 

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(5) RCT A 402950-18-9, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT M 37394-93-7

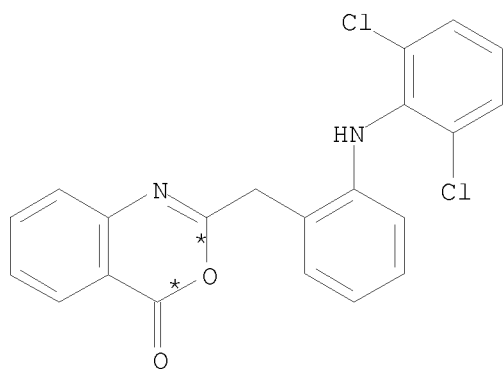
SOL 67-56-1 MeOH

CON reflux

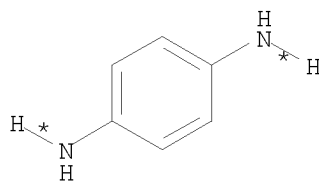
PRO N 945486-77-1

RX(6) OF 48 A + B + O ==> P

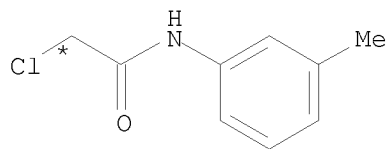
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A



B



O

(6)  $\longrightarrow$

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(6) RCT A 402950-18-9, B 106-50-3

STAGE(1)

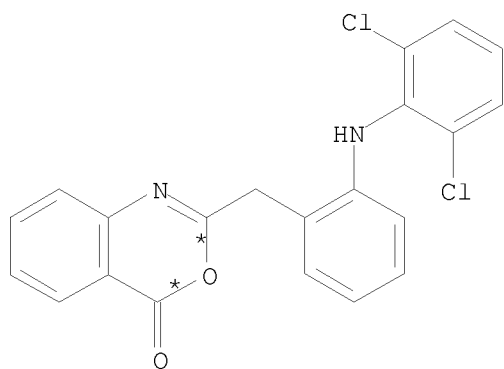
SOL 110-86-1 Pyridine  
CON reflux

STAGE(2)

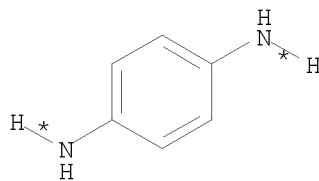
RCT O 32428-61-8  
SOL 67-56-1 MeOH  
CON reflux

PRO P 945486-78-2

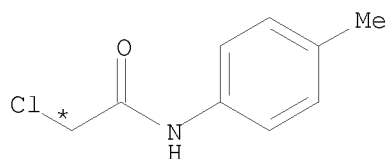
RX(7) OF 48 A + B + Q ==> R



A



B



Q



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(7) RCT A 402950-18-9, B 106-50-3

STAGE(1)

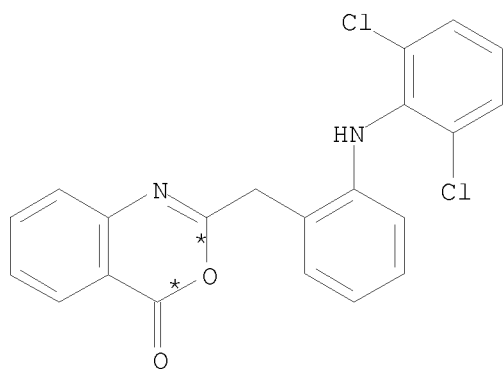
SOL 110-86-1 Pyridine  
CON reflux

STAGE(2)

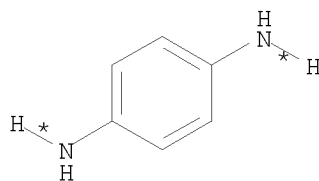
RCT Q 16634-82-5  
SOL 67-56-1 MeOH  
CON reflux

PRO R 945486-79-3

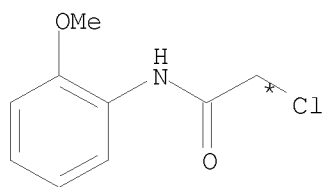
RX(8) OF 48 A + B + S ==> T



A



B



S



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(8) RCT A 402950-18-9, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT S 55860-22-5

SOL 67-56-1 MeOH

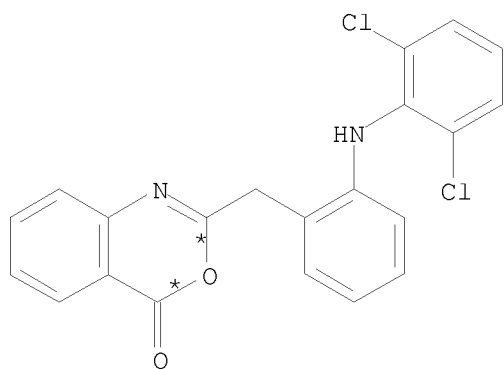
CON reflux

PRO T 945486-80-6

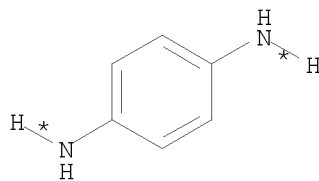
RX(9) OF 48 A + B + U ==> V



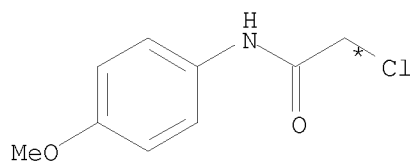
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A



B



U



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(9) RCT A 402950-18-9, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine  
CON reflux

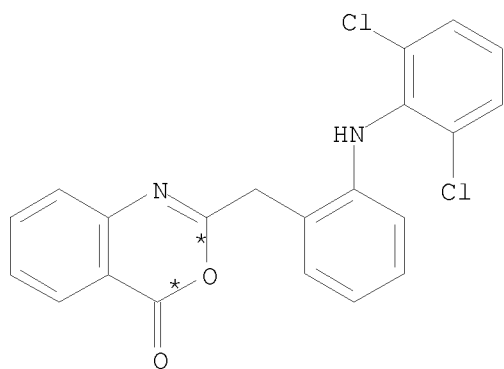
STAGE(2)

RCT U 22303-36-2  
SOL 67-56-1 MeOH  
CON reflux

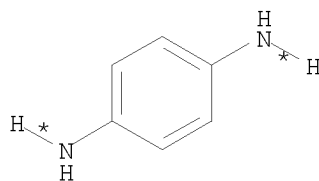
PRO V 945486-81-7

RX(10) OF 48 A + B + W ==> X

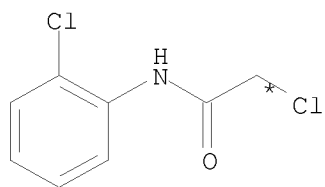
10/ 562,112



A



B



W



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(10) RCT A 402950-18-9, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT W 3289-76-7

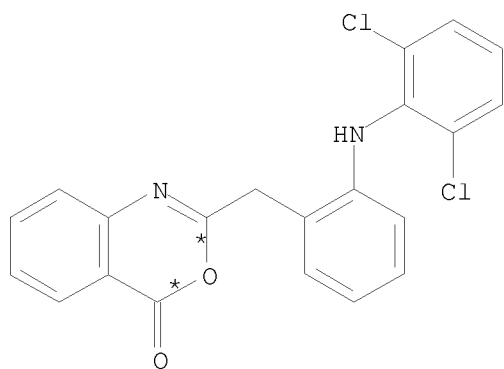
SOL 67-56-1 MeOH

CON reflux

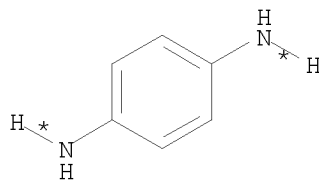
PRO X 945486-82-8

RX(11) OF 48 A + B + Y ==> Z

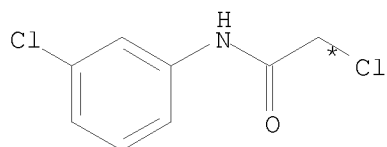
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A



B



Y

(11)  $\longrightarrow$

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(11) RCT A 402950-18-9, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

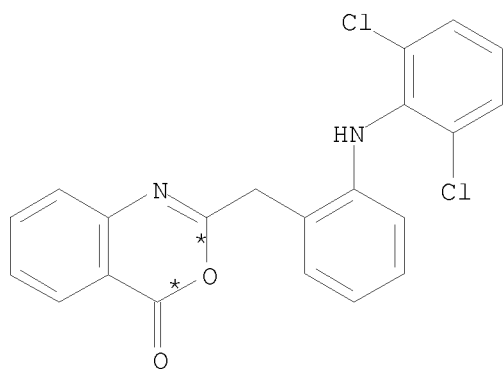
RCT Y 2564-05-8

SOL 67-56-1 MeOH

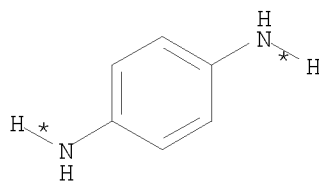
CON reflux

PRO Z 945486-83-9

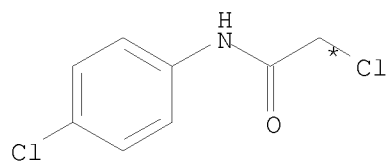
RX(12) OF 48 A + B + AA ==> AB



A



B



AA

(12)  $\longrightarrow$ 

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(12) RCT A 402950-18-9, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

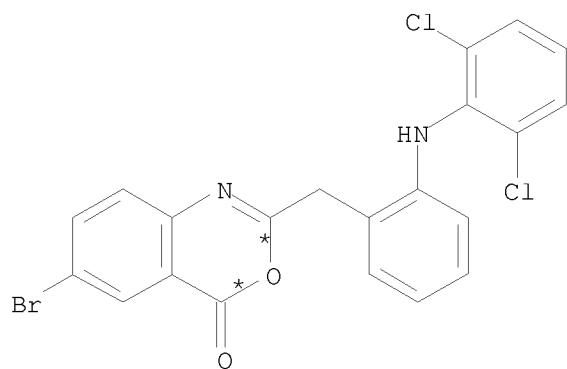
RCT AA 3289-75-6

SOL 67-56-1 MeOH

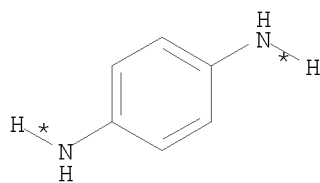
CON reflux

PRO AB 945486-84-0

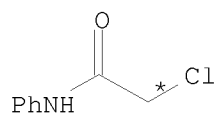
RX(13) OF 48 AC + B + C ==> AD



AC

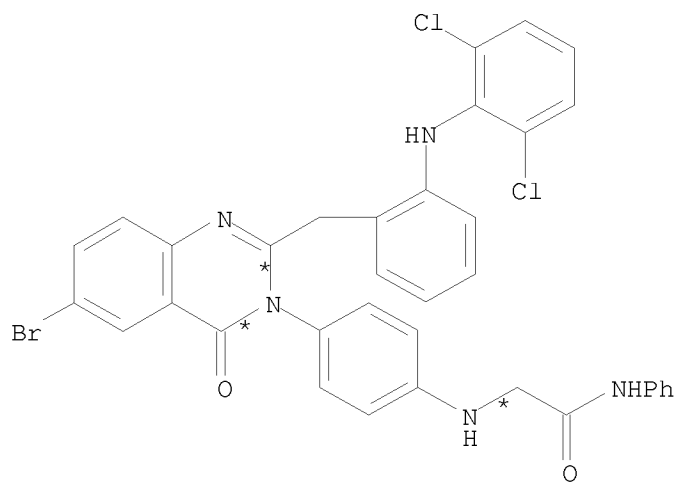


B



C

(13) →



AD

YIELD 39%

RX(13) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT C 587-65-5

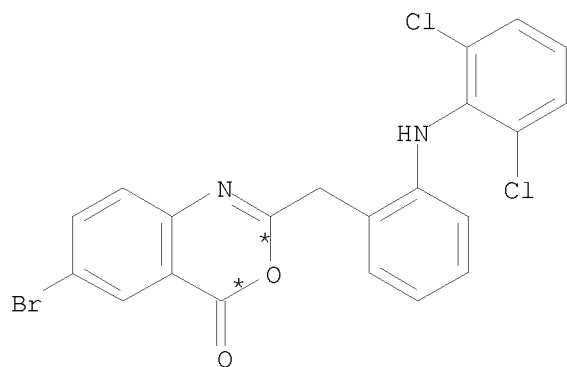
SOL 67-56-1 MeOH

10/ 562,112

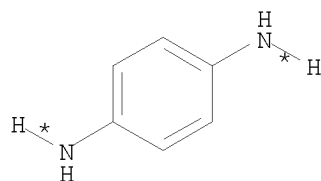
CON reflux

PRO AD 945486-85-1

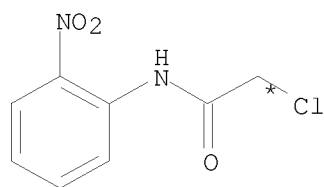
RX(14) OF 48 AC + B + G ==> AE



AC



B



G



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(14) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT G 10147-70-3

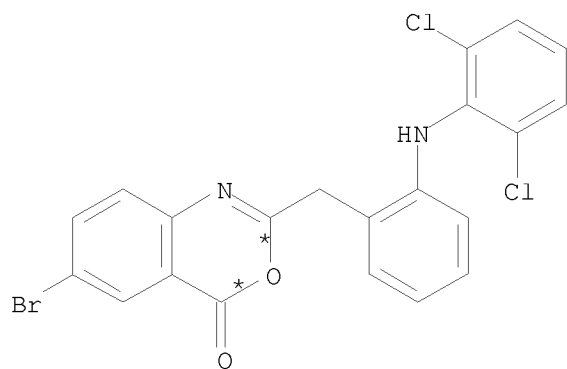
SOL 67-56-1 MeOH

CON reflux

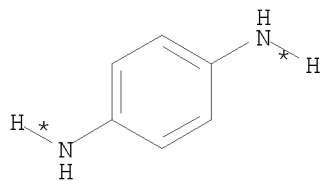
PRO AE 945486-86-2

RX(15) OF 48 AC + B + I ==> AF

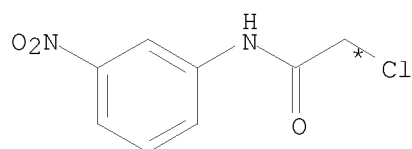
10/ 562,112



AC



B



I

(15)  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(15) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT I 10147-71-4

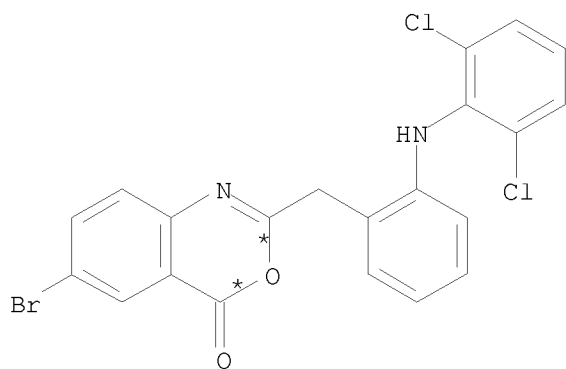
SOL 67-56-1 MeOH

CON reflux

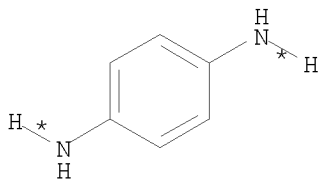
PRO AF 945486-87-3

RX(16) OF 48 AC + B + K ==> AG

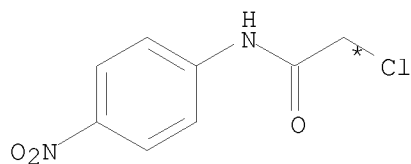
10/ 562,112



AC



B



K

(16)  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(16) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT K 17329-87-2

SOL 67-56-1 MeOH

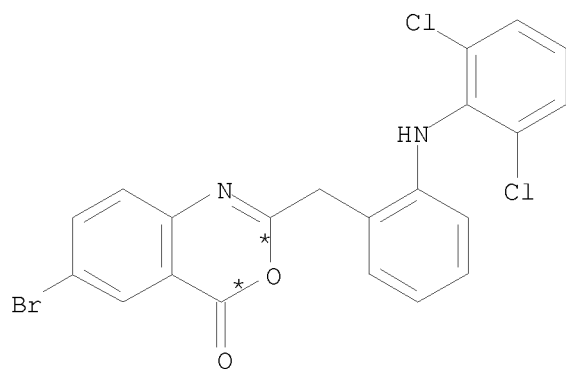
CON reflux

PRO AG 945486-88-4

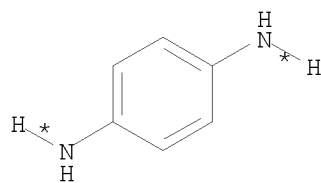
RX(17) OF 48 AC + B + M ==> AH



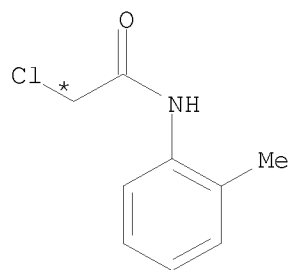
10/ 562,112



AC



B



M



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(17) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT M 37394-93-7

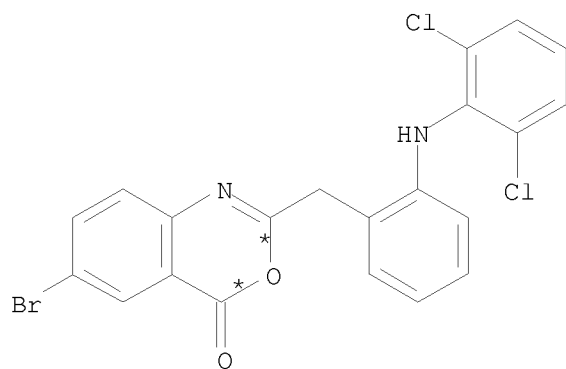
SOL 67-56-1 MeOH

CON reflux

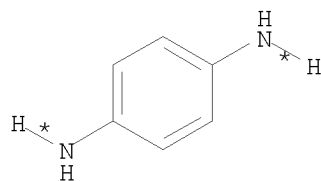
PRO AH 945486-89-5

RX(18) OF 48 AC + B + O ==> AI

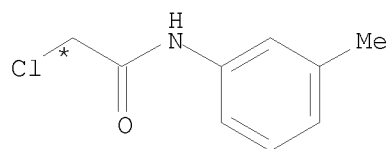
10/ 562,112



AC



B



O

(18)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(18) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine  
CON reflux

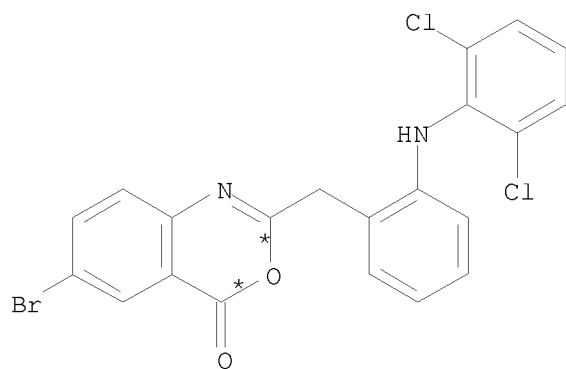
STAGE(2)

RCT O 32428-61-8  
SOL 67-56-1 MeOH  
CON reflux

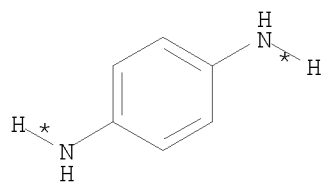
PRO AI 945486-90-8

RX(19) OF 48 AC + B + Q ==> AJ

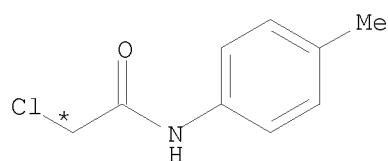
10/ 562,112



AC



B



Q



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(19) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine  
CON reflux

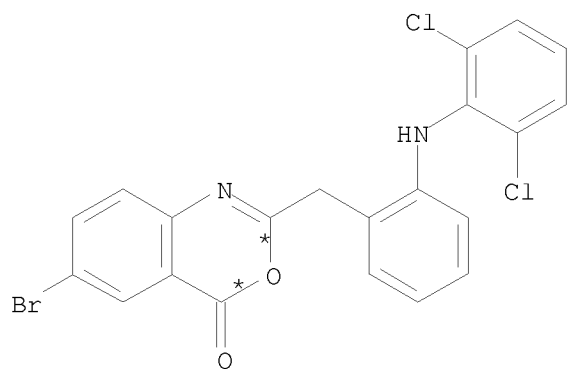
STAGE(2)

RCT Q 16634-82-5  
SOL 67-56-1 MeOH  
CON reflux

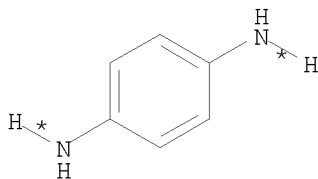
PRO AJ 945486-91-9

RX(20) OF 48 AC + B + S ==> AK

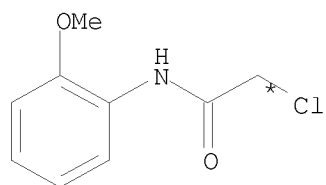
10/ 562,112



AC



B



S

(20)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(20) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT S 55860-22-5

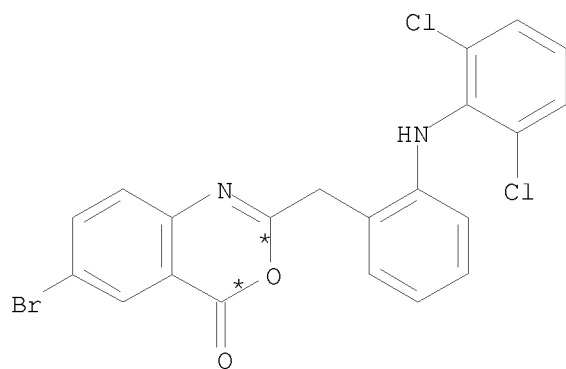
SOL 67-56-1 MeOH

CON reflux

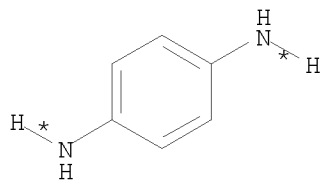
PRO AK 945486-92-0

RX(21) OF 48 AC + B + U ==> AL

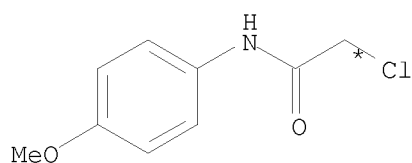
10/ 562,112



AC



B



U



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(21) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine  
CON reflux

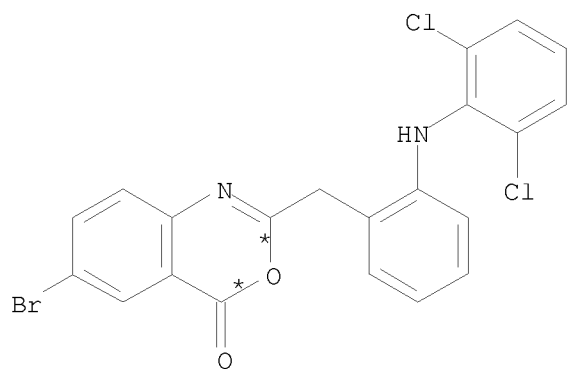
STAGE(2)

RCT U 22303-36-2  
SOL 67-56-1 MeOH  
CON reflux

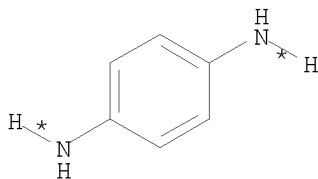
PRO AL 945486-93-1

RX(22) OF 48 AC + B + W ==> AM

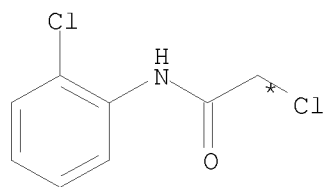
10/ 562,112



AC



B



W



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(22) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT W 3289-76-7

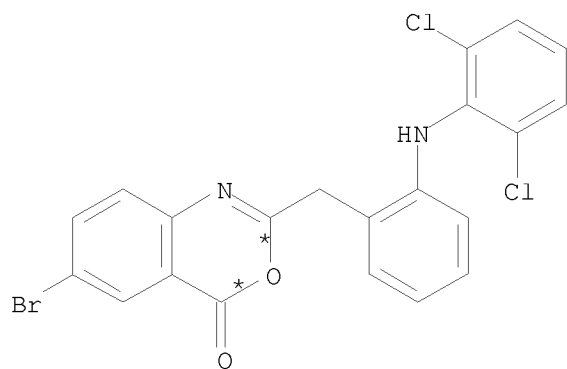
SOL 67-56-1 MeOH

CON reflux

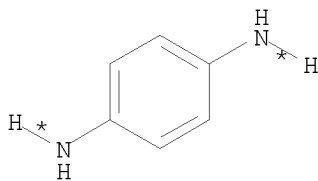
PRO AM 945486-94-2

RX(23) OF 48 AC + B + Y ==> AN

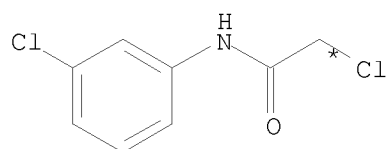
10/ 562,112



AC



B



Y



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(23) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine  
CON reflux

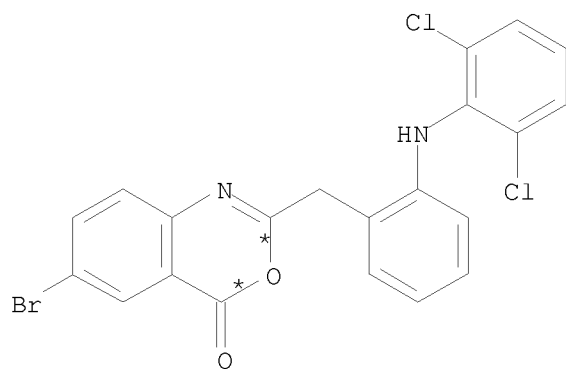
STAGE(2)

RCT Y 2564-05-8  
SOL 67-56-1 MeOH  
CON reflux

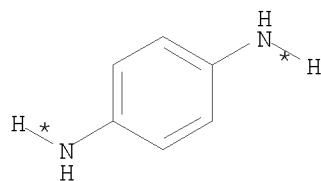
PRO AN 945486-95-3

RX(24) OF 48 AC + B + AA ==> AO

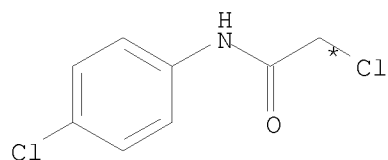
10/ 562,112



AC



B



AA

(24)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(24) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT AA 3289-75-6

SOL 67-56-1 MeOH

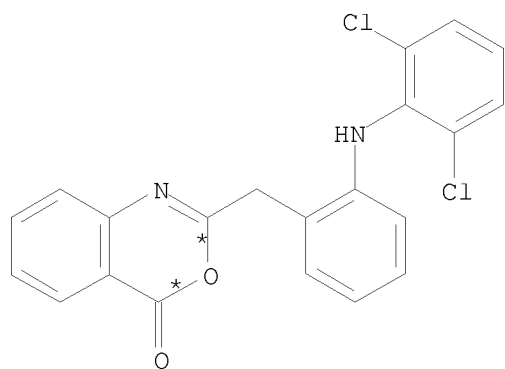
CON reflux

PRO AO 945486-96-4

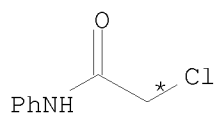
RX(25) OF 48 A + C ==> AP



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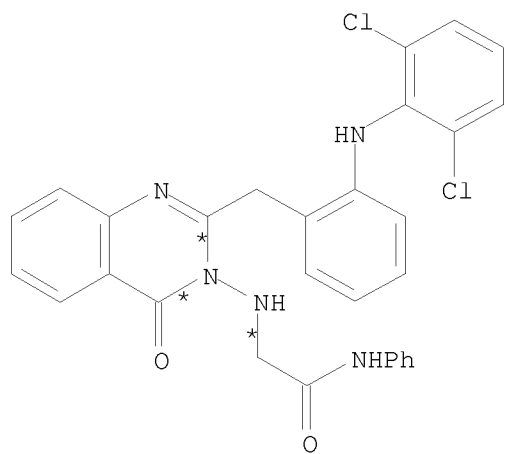


A



C

(25)  $\longrightarrow$



AP

YIELD 40%

RX(25) RCT A 402950-18-9

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT C 587-65-5

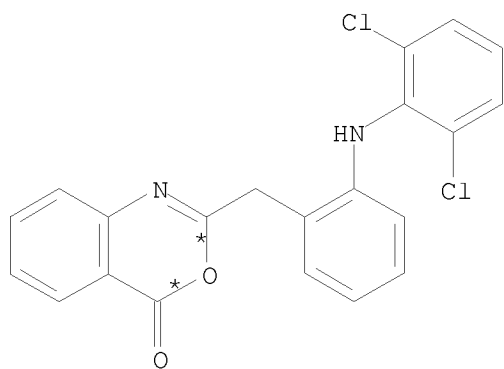
SOL 67-56-1 MeOH

CON reflux

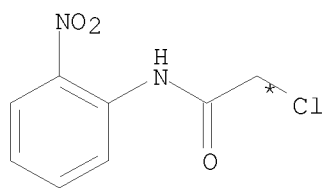
PRO AP 945486-97-5

RX(26) OF 48 A + G ==> AR

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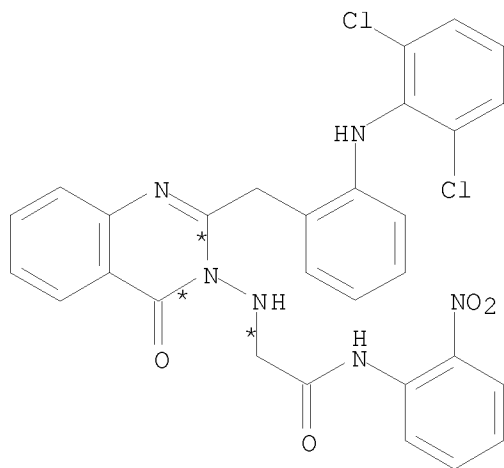


A



G

(26)



AR

YIELD 46%

RX(26) RCT A 402950-18-9

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT G 10147-70-3

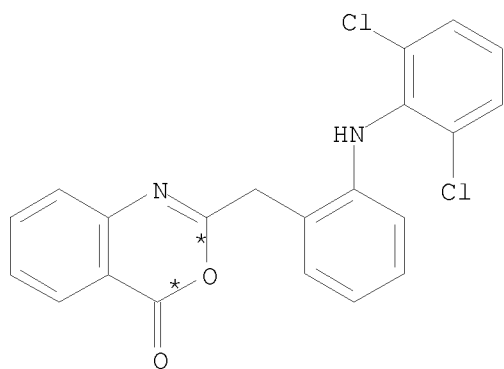
SOL 67-56-1 MeOH

CON reflux

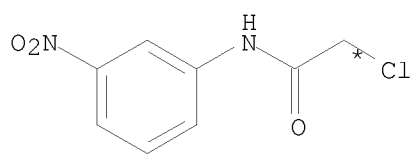
PRO AR 945486-98-6

RX(27) OF 48 A + I ==> AS

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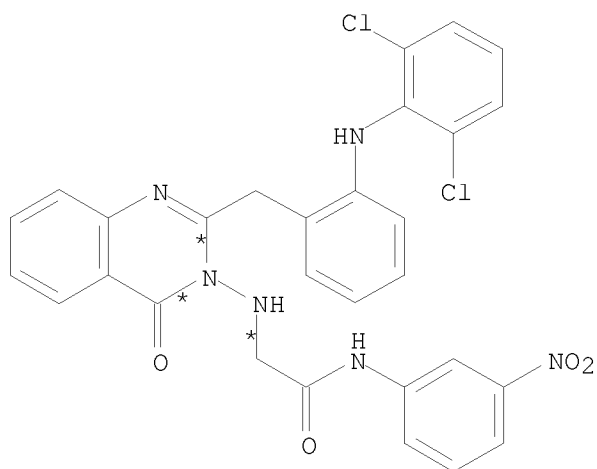


A



I

(27)  
→



AS

YIELD 44%

RX(27) RCT A 402950-18-9

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT I 10147-71-4

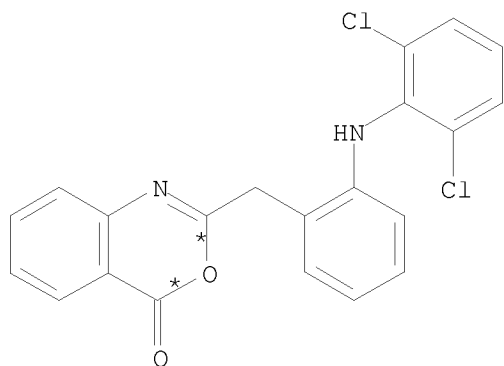
SOL 67-56-1 MeOH

CON reflux

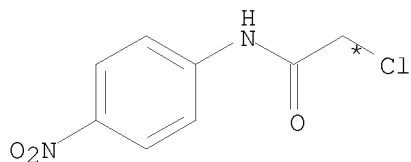
PRO AS 945486-99-7

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RX(28) OF 48      A + K ==> AT

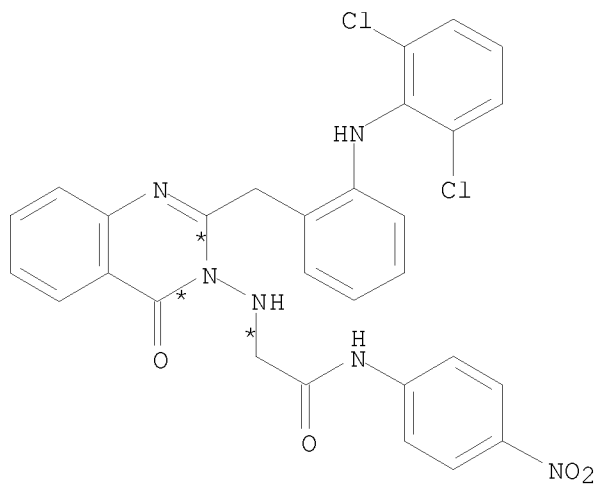


A



K

(28)  
→



AT

YIELD 44%

RX(28)      RCT    A 402950-18-9

STAGE(1)

RGT    AQ 7803-57-8 N2H4-H2O

SOL    110-86-1 Pyridine

CON    reflux

STAGE(2)

RCT    K 17329-87-2

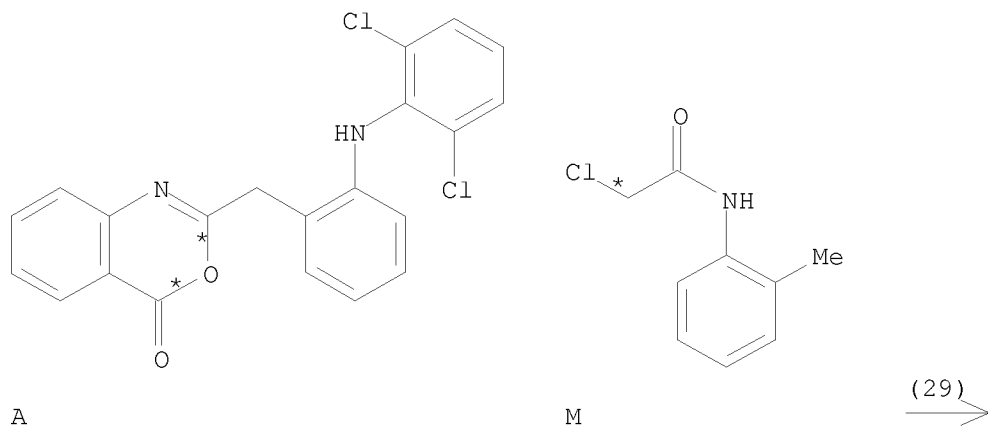
SOL    67-56-1 MeOH

CON    reflux

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PRO AT 945487-00-3

RX(29) OF 48 A + M ==> AU



AU  
YIELD 56%

RX(29) RCT A 402950-18-9

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O  
SOL 110-86-1 Pyridine  
CON reflux

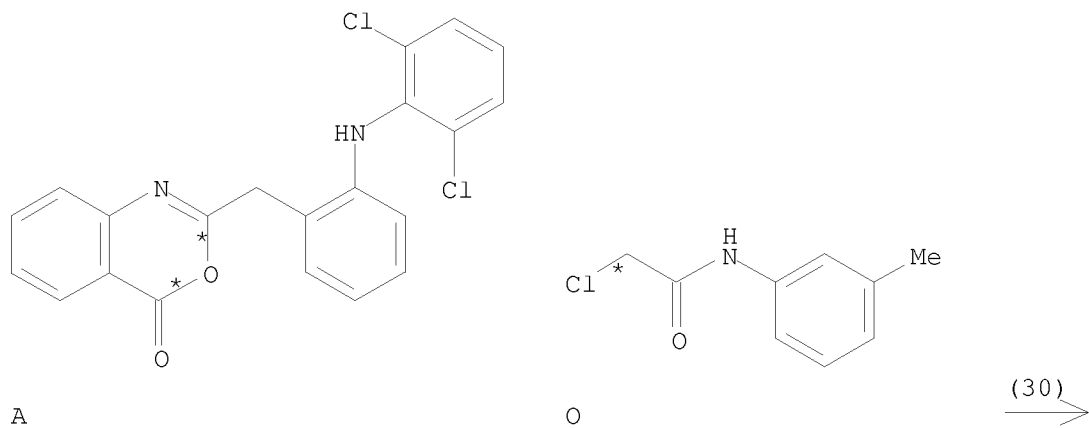
STAGE(2)

RCT M 37394-93-7  
SOL 67-56-1 MeOH  
CON reflux

PRO AU 945487-01-4

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RX(30) OF 48      A + O ==> AV



AV  
YIELD 51%

RX(30)      RCT    A 402950-18-9

STAGE(1)

RGT    AQ 7803-57-8 N2H4-H2O

SOL    110-86-1 Pyridine

CON    reflux

STAGE(2)

RCT    O 32428-61-8

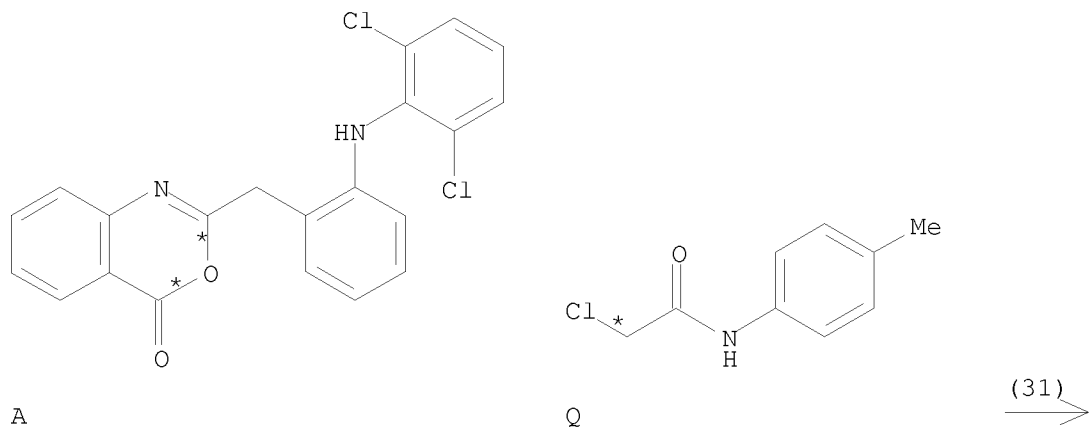
SOL    67-56-1 MeOH

CON    reflux

PRO    AV 945487-02-5

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RX(31) OF 48      A + Q ==> AW



AW  
YIELD 39%

RX(31)      RCT    A 402950-18-9

STAGE(1)

RGT    AQ 7803-57-8 N2H4-H2O  
SOL    110-86-1 Pyridine  
CON    reflux

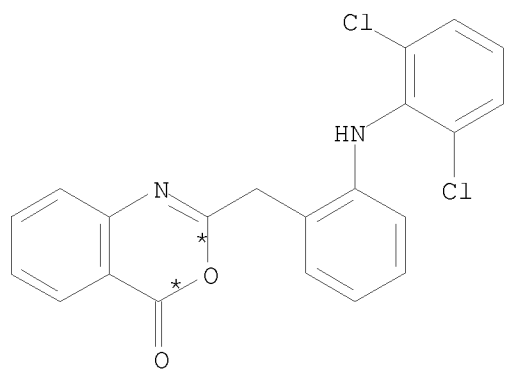
STAGE(2)

RCT    Q 16634-82-5  
SOL    67-56-1 MeOH  
CON    reflux

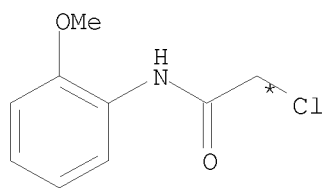
PRO    AW 945487-03-6

RX(32) OF 48      A + S ==> AX

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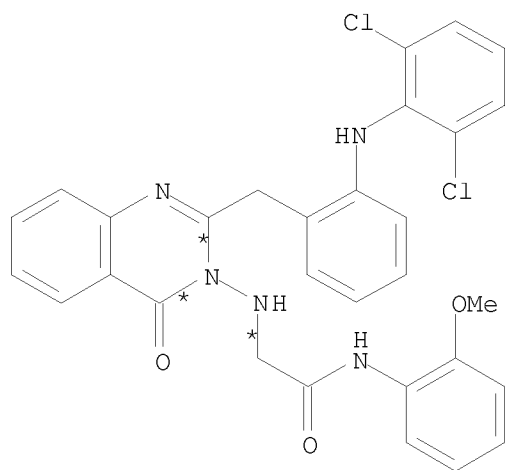


A



S

(32)  $\rightarrow$



AX

YIELD 62%

RX(32) RCT A 402950-18-9

STAGE(1)

RGT AQ 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT S 55860-22-5

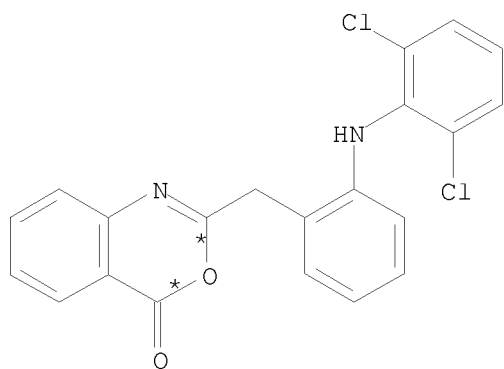
SOL 67-56-1 MeOH

CON reflux

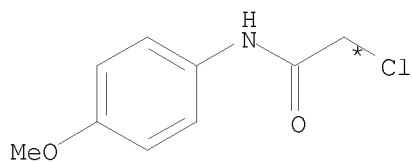
PRO AX 945487-04-7

RX(33) OF 48 A + U ==> AY



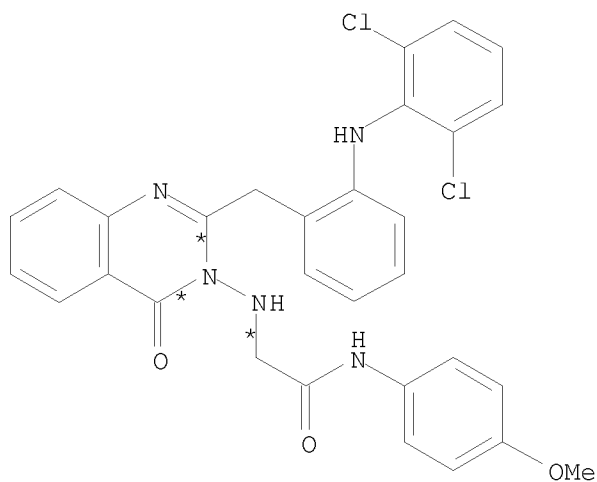


A



U

(33) →



AY

YIELD 63%

RX(33) RCT A 402950-18-9

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O  
 SOL 110-86-1 Pyridine  
 CON reflux

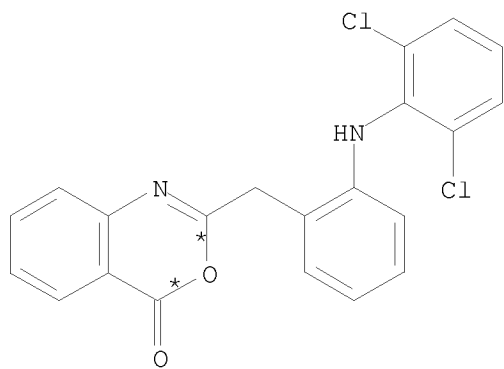
STAGE(2)

RCT U 22303-36-2  
 SOL 67-56-1 MeOH  
 CON reflux

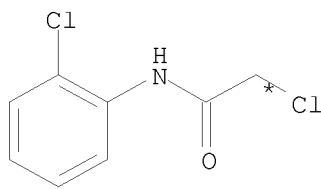
PRO AY 945487-05-8

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RX(34) OF 48      A + W ==> AZ

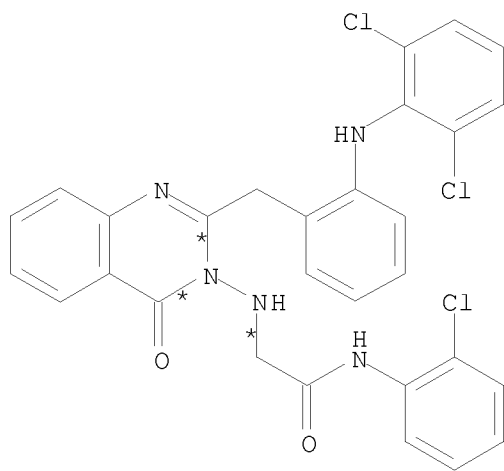


A



W

(34) 



AZ

YIELD 46%

RX(34)      RCT    A 402950-18-9

STAGE(1)

RGT    AQ 7803-57-8 N2H4-H2O

SOL    110-86-1 Pyridine

CON    reflux

STAGE(2)

RCT    W 3289-76-7

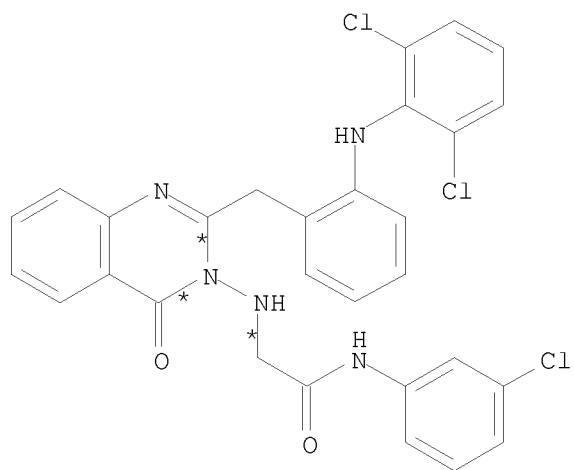
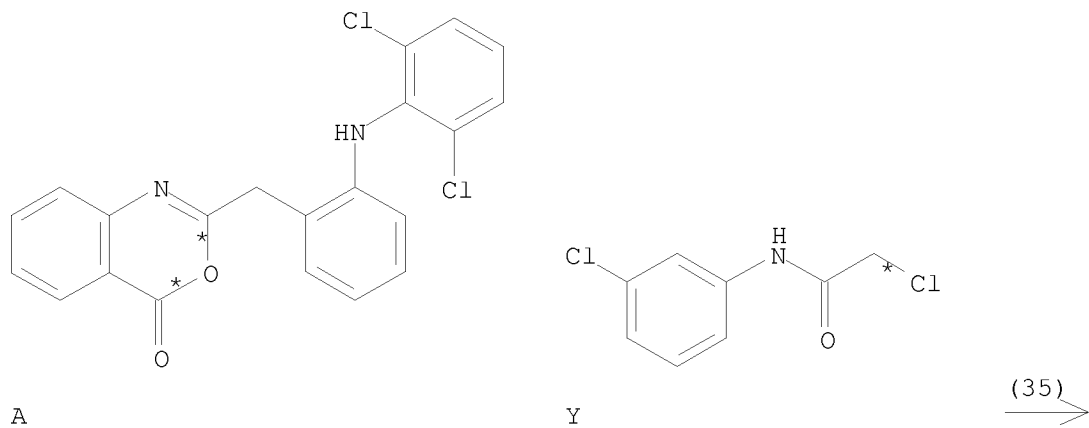
SOL    67-56-1 MeOH

CON    reflux

PRO    AZ 945487-06-9

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RX(35) OF 48      A + Y ==> BA



BA  
YIELD 45%

RX(35)      RCT    A 402950-18-9

STAGE(1)

RGT    AQ 7803-57-8 N2H4-H2O  
SOL    110-86-1 Pyridine  
CON    reflux

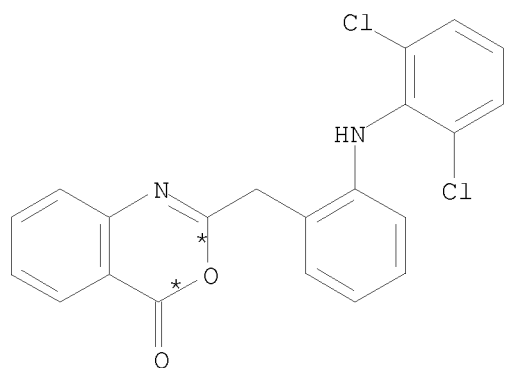
STAGE(2)

RCT    Y 2564-05-8  
SOL    67-56-1 MeOH  
CON    reflux

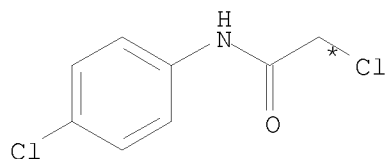
PRO    BA 945487-07-0

RX(36) OF 48      A + AA ==> BB

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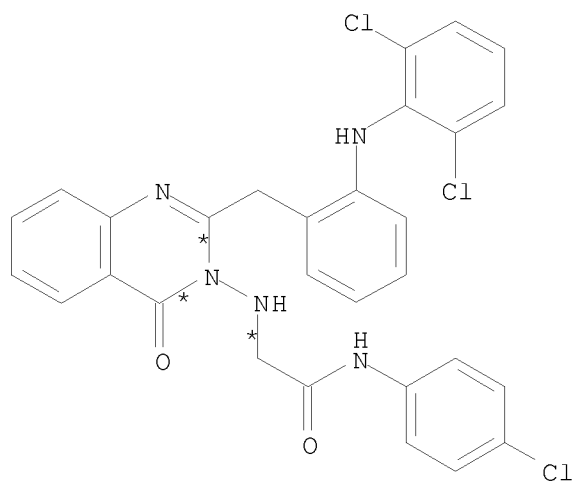


A



AA

(36)  $\longrightarrow$



BB

YIELD 45%

RX(36) RCT A 402950-18-9

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT AA 3289-75-6

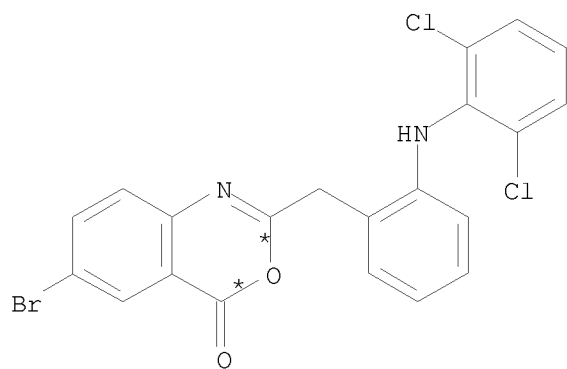
SOL 67-56-1 MeOH

CON reflux

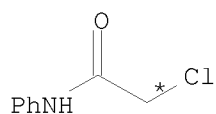
PRO BB 945487-08-1

RX(37) OF 48 AC + C ==> BC

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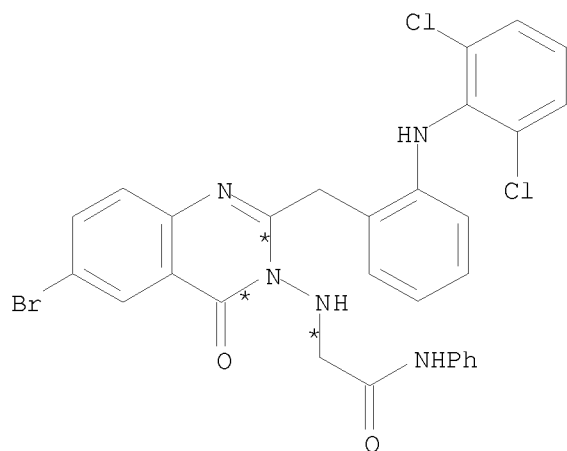


AC



C

(37)  $\longrightarrow$



BC

YIELD 42%

RX(37) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT C 587-65-5

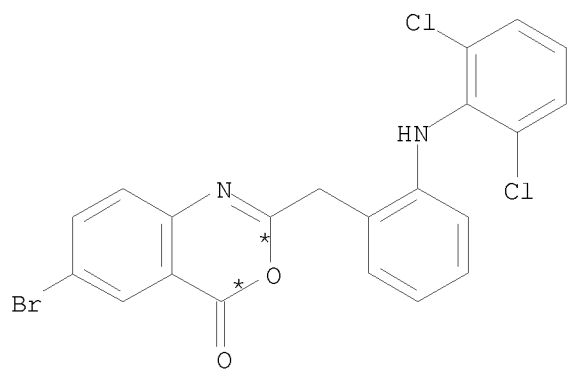
SOL 67-56-1 MeOH

CON reflux

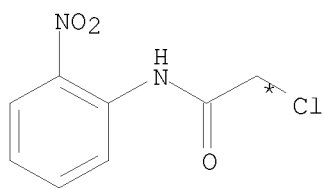
PRO BC 945487-09-2

RX(38) OF 48 AC + G ==> BD

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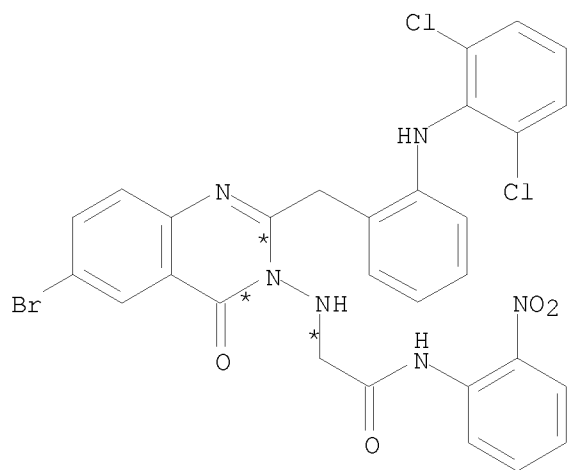


AC



G

(38)  $\longrightarrow$



BD

YIELD 47%

RX(38) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT G 10147-70-3

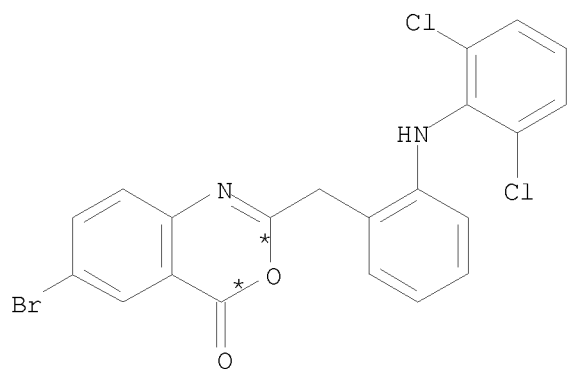
SOL 67-56-1 MeOH

CON reflux

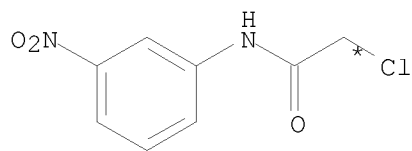
PRO BD 945487-10-5

RX(39) OF 48 AC + I ==> BE

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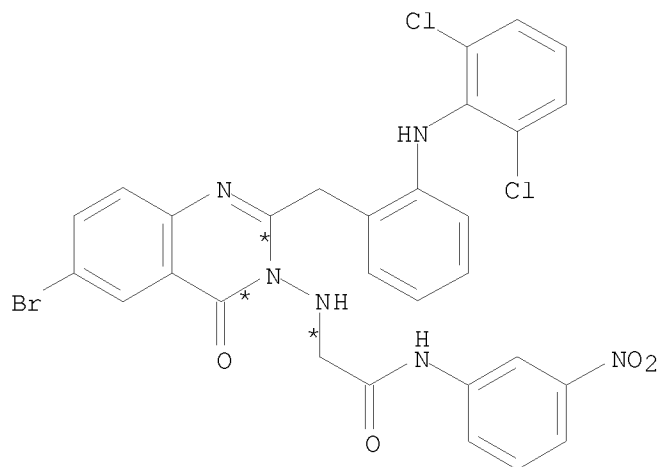


AC



I

(39)  
→



BE  
YIELD 49%

RX(39) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O  
SOL 110-86-1 Pyridine  
CON reflux

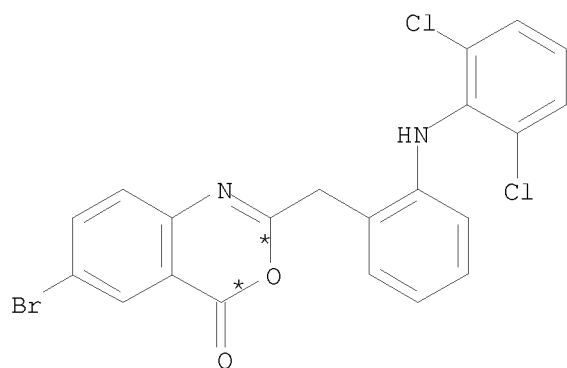
STAGE(2)

RCT I 10147-71-4  
SOL 67-56-1 MeOH  
CON reflux

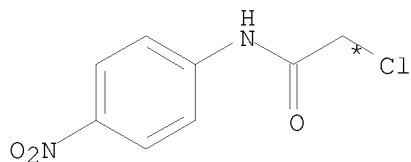
PRO BE 945487-11-6

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RX(40) OF 48 AC + K ==> BF

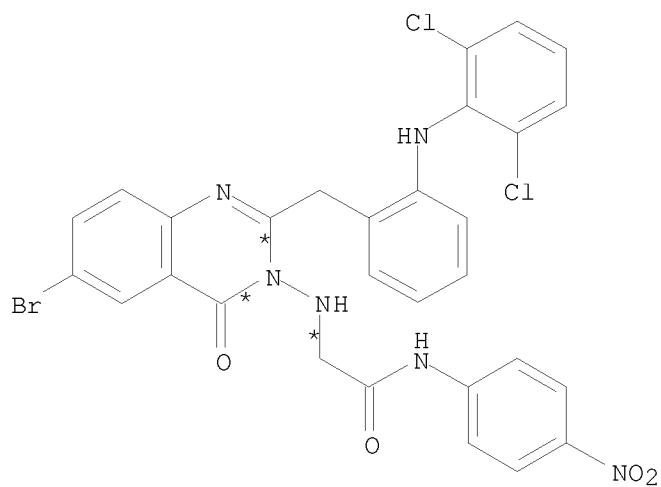


AC



K

(40)  
=>



BF

YIELD 41%

RX(40) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 110-86-1 Pyridine  
CON reflux

STAGE(2)

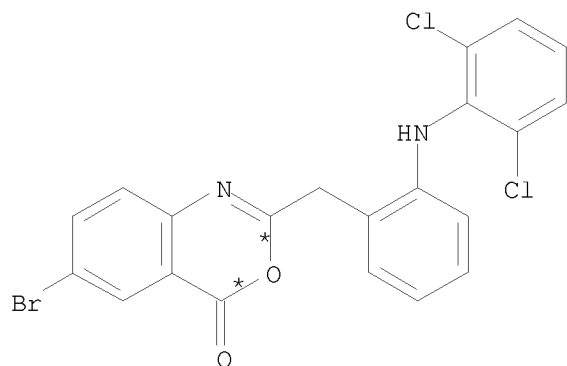
RCT K 17329-87-2  
SOL 67-56-1 MeOH  
CON reflux



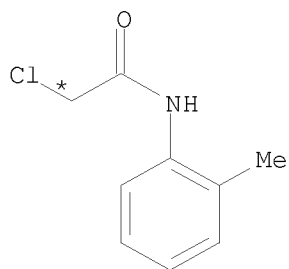
10/ 562,112

PRO BF 945487-12-7

RX(41) OF 48 AC + M ==> BG

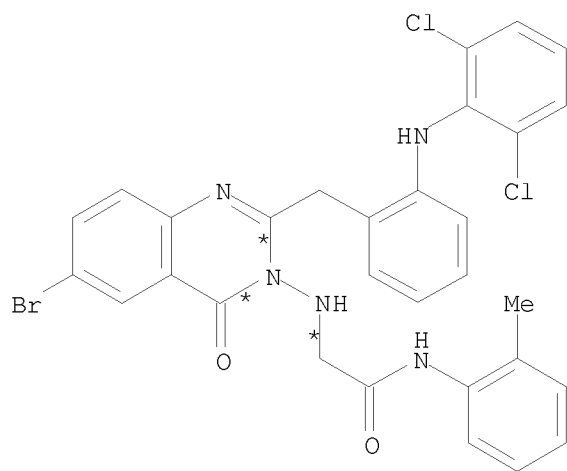


AC



M

(41)



BG  
YIELD 33%

RX(41) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O  
SOL 110-86-1 Pyridine  
CON reflux

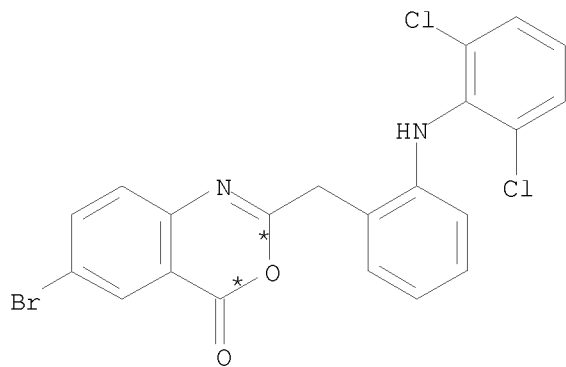
STAGE(2)

RCT M 37394-93-7  
SOL 67-56-1 MeOH  
CON reflux

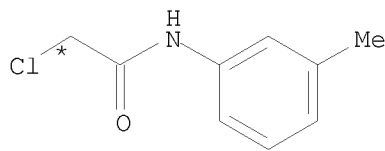
PRO BG 945487-13-8

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RX(42) OF 48 AC + O ==> BH

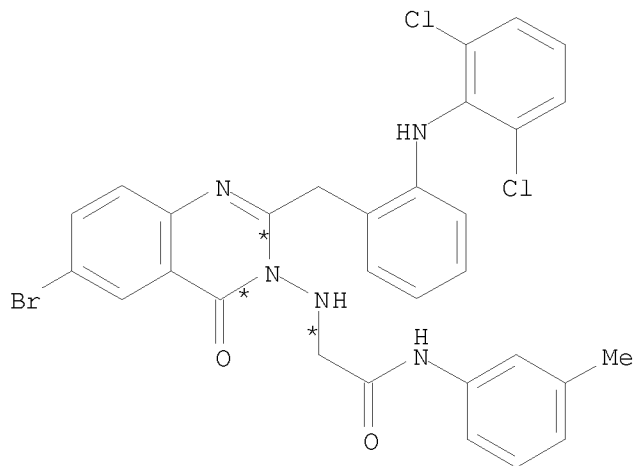


AC



O

(42) 



BH  
YIELD 39%

RX(42) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O  
SOL 110-86-1 Pyridine  
CON reflux

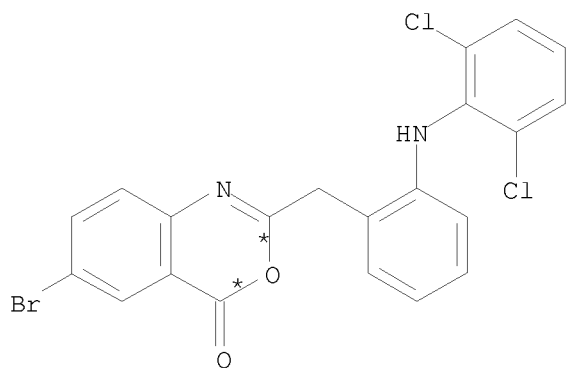
STAGE(2)

RCT O 32428-61-8  
SOL 67-56-1 MeOH  
CON reflux

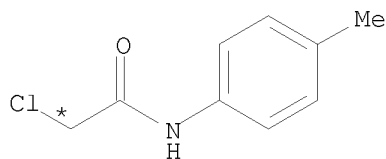
10/ 562,112

PRO BH 945487-14-9

RX(43) OF 48 AC + Q ==> BI

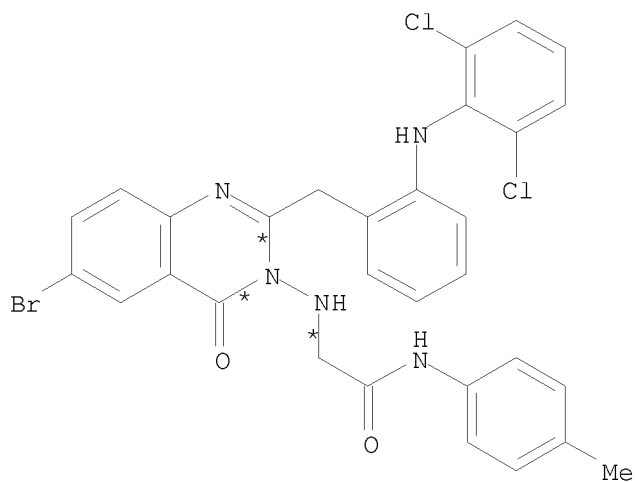


AC



Q

(43) 



BI

YIELD 38%

RX(43) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

STAGE(2)

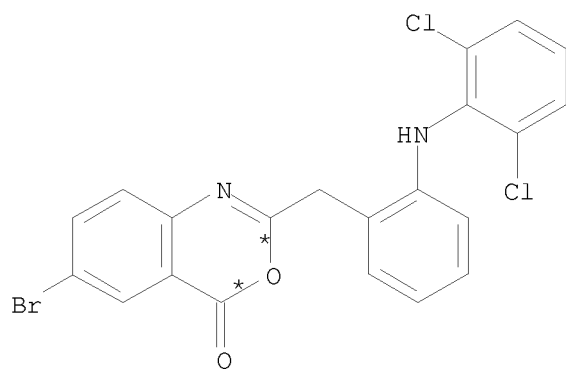
RCT Q 16634-82-5

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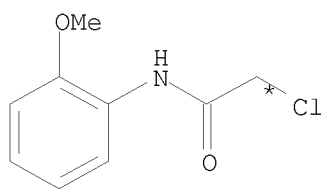
SOL 67-56-1 MeOH

PRO BI 945487-15-0

RX(44) OF 48 AC + S ==> BJ

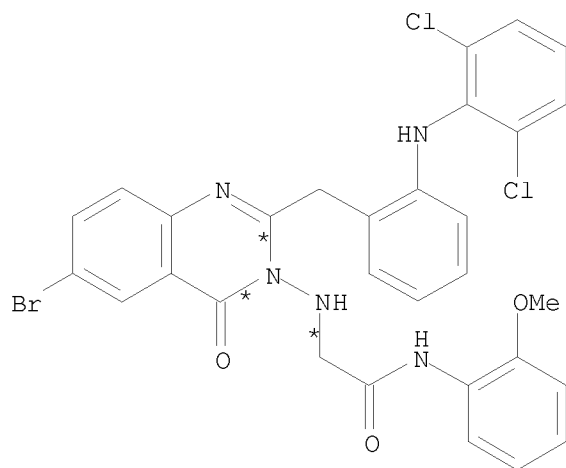


AC



S

(44) 



BJ

YIELD 63%

RX(44) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

STAGE(2)

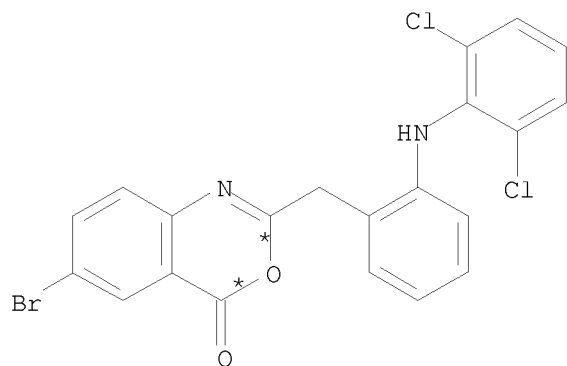
RCT S 55860-22-5

SOL 67-56-1 MeOH

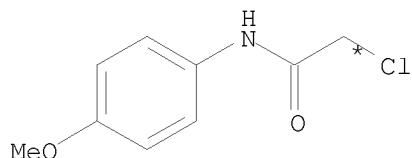
PRO BJ 945487-16-1

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RX(45) OF 48 AC + U ==> BK

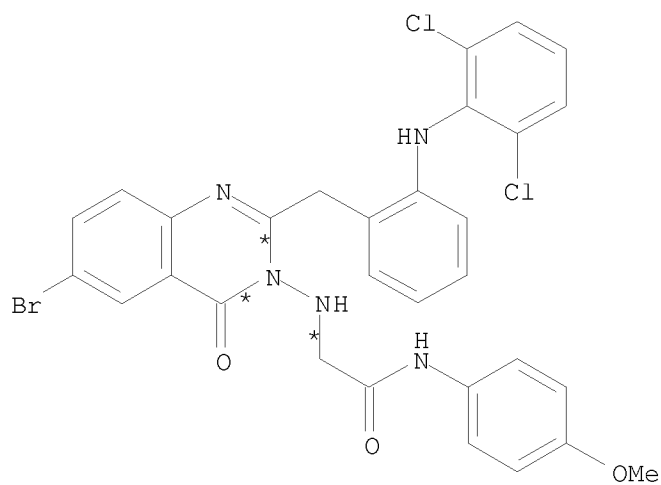


AC



U

(45)  
=>



BK

YIELD 66%

RX(45) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

STAGE(2)

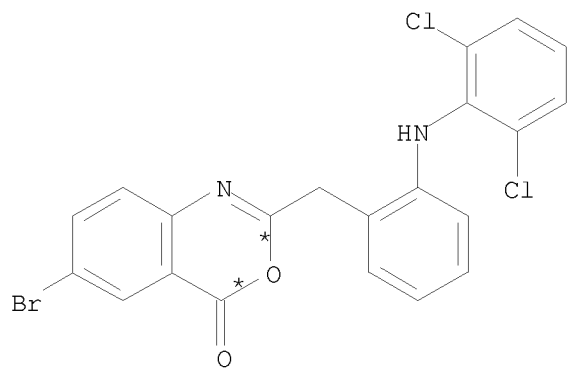
RCT U 22303-36-2

SOL 67-56-1 MeOH

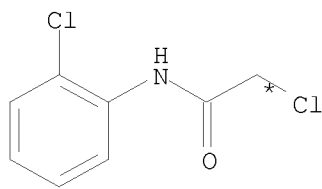
PRO BK 945487-17-2

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RX(46) OF 48      AC   +   W   ==>   BL

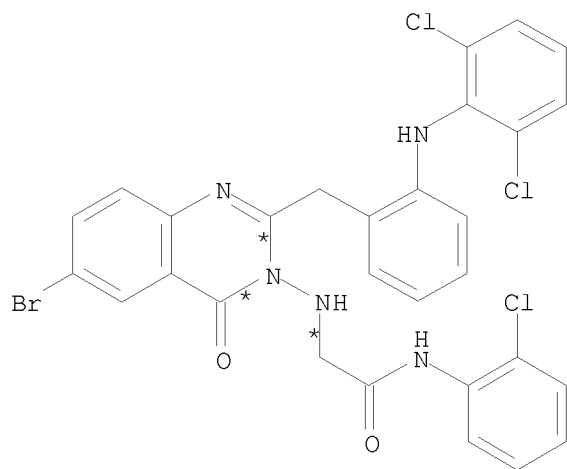


AC



W

(46)



BL

YIELD 36%

RX(46)      RCT    AC 945487-25-2

STAGE(1)

RGT    AQ 7803-57-8 N2H4-H2O

SOL    110-86-1 Pyridine

STAGE(2)

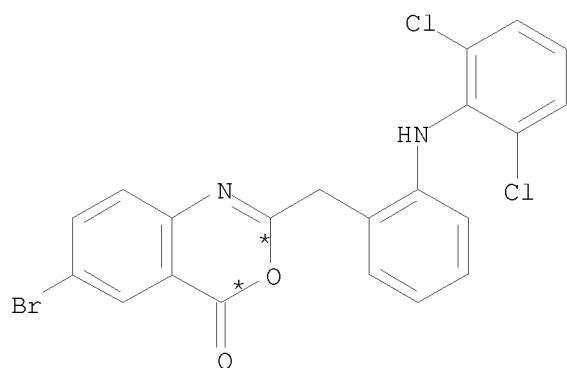
RCT    W 3289-76-7

SOL    67-56-1 MeOH

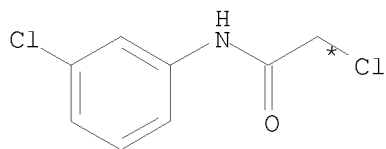
PRO    BL 945487-18-3

RX(47) OF 48      AC   +   Y   ==>   BM

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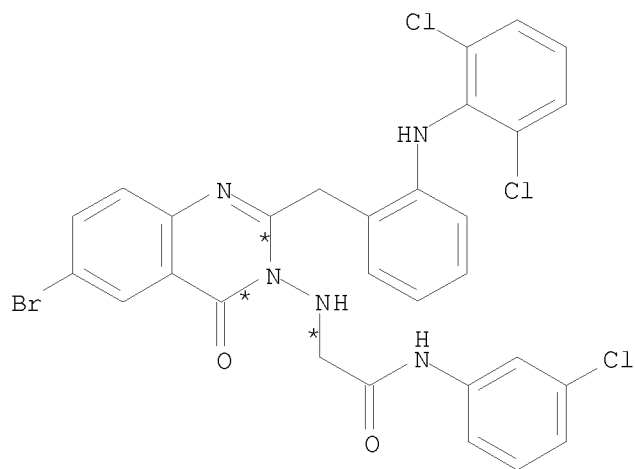


AC



Y

(47)  
→



BM  
YIELD 37%

RX(47) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

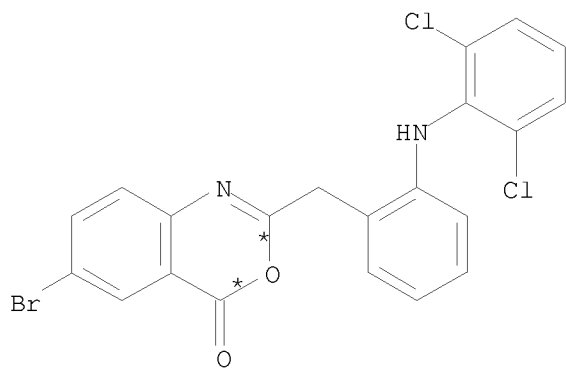
STAGE(2)

RCT Y 2564-05-8

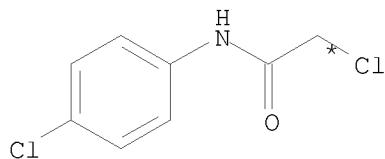
SOL 67-56-1 MeOH

PRO BM 945487-19-4

RX(48) OF 48 AC + AA ==> BN

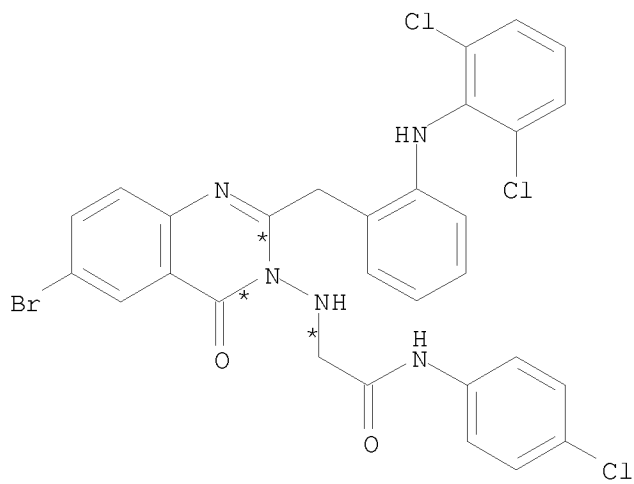


AC



AA

(48)



BN  
YIELD 40%

RX (48) RCT AC 945487-25-2

STAGE ( 1 )

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

STAGE (2)

RCT AA 3289-75-6

SOL 67-56-1 MeOH

PRO BN 945487-22-9



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REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 18 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 147:211826 CASREACT

TITLE: Discovery and optimization of a series of quinazolinone-derived antagonists of CXCR3

AUTHOR(S): Johnson, Michael; Li, An-Rong; Liu, Jiwen; Fu, Zice; Zhu, Liusheng; Miao, Shichang; Wang, Xuemei; Xu, Qingge; Huang, Alan; Marcus, Andrew; Xu, Feng; Ebsworth, Karen; Sablan, Emmanuel; Danao, Jay; Kumer, Jeff; Dairaghi, Dan; Lawrence, Chris; Sullivan, Tim; Tonn, George; Schall, Thomas; Collins, Tassie; Medina, Julio

CORPORATE SOURCE: Amgen Inc., South San Francisco, CA, 94080, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(12), 3339-3343

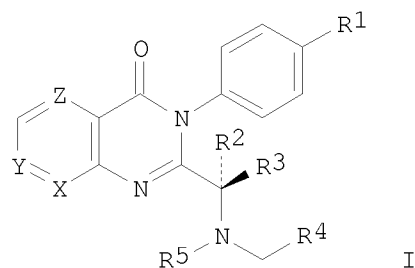
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

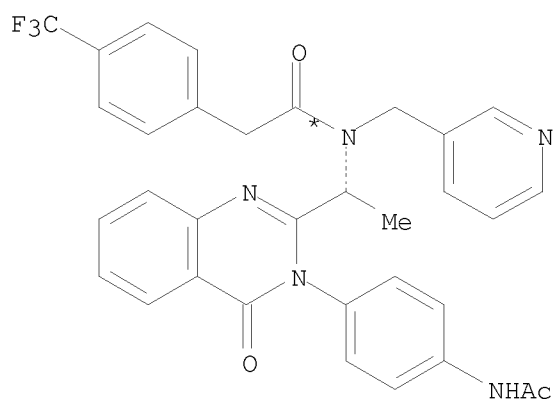
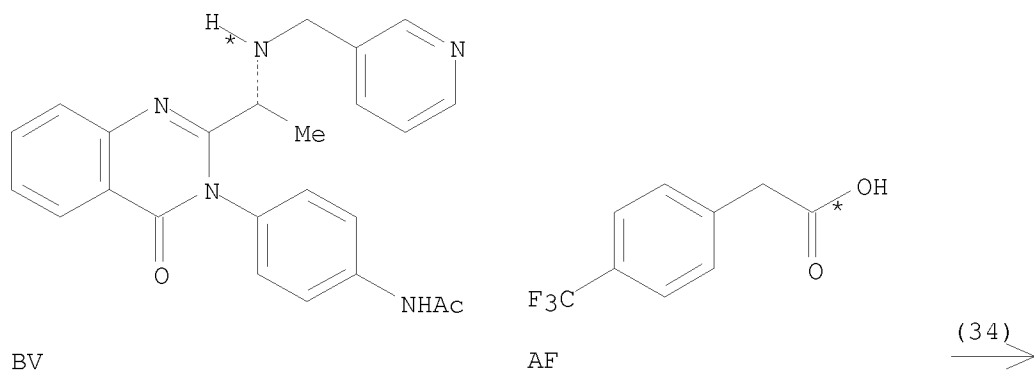
GI



AB A series of quinazolinone-derived inhibitors of the CXCR3 receptor I (X, Y, Z = CH, N; R1 = H, F, Cl, EtO, MeC.tplbond.C, etc.; R2 = R3 = H, Me; R2 = H, R3 = Me, Et, Ph; R4 = Me2NCH2, EtOCH2, 3-pyridyl, etc.; R5 = n-octyl, 4-F3CC6H4CH2CO, n-C8H17SO2, etc.) have been synthesized and their affinity for the receptor evaluated. These compds. were evaluated in a 125I-IP10 displacement assay and in in vitro cell migration assays to IP10, ITAC, and MIG using human peripheral blood mononuclear cells.

RX(34) OF 342 ...BV + AF ==> BW

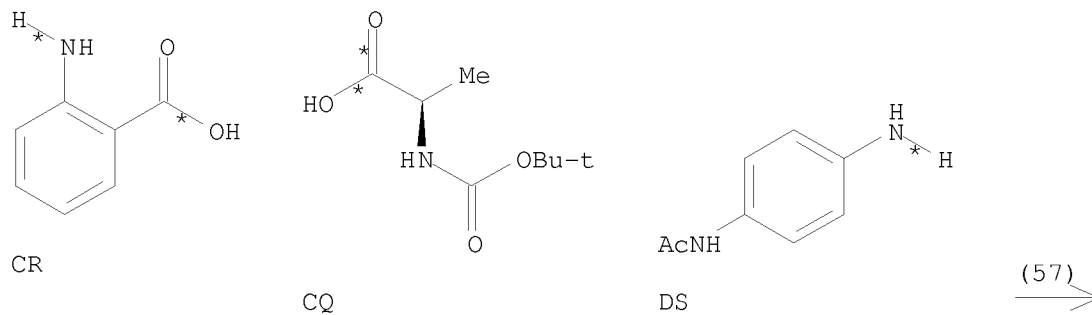
10/ 562,112



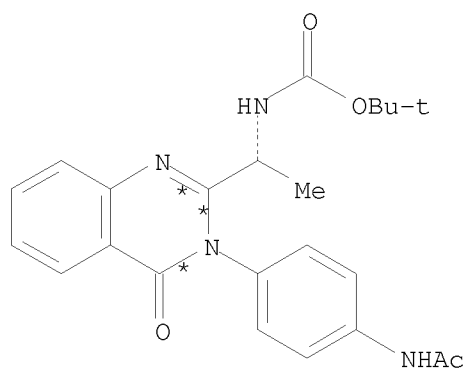
YIELD 90%

RX(34) RCT BV 944915-81-5, AF 32857-62-8  
 RGT D 2592-95-2 1-Benzotriazolol, E 25952-53-8 EDAP  
 PRO BW 944915-21-3  
 SOL 68-12-2 DMF  
 CON 1 hour, room temperature

RX(57) OF 342 CR + CQ + DS ==> DT...



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DT  
YIELD 50%

RX(57) RCT CR 118-92-3, CQ 7764-95-6

STAGE(1)

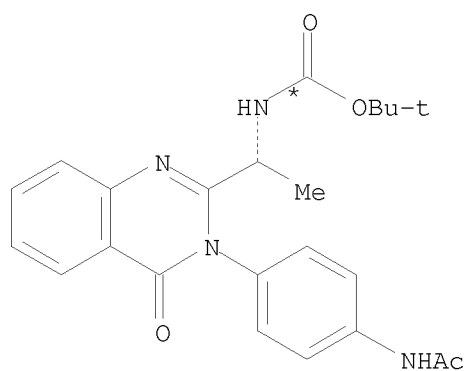
RGT U 110-86-1 Pyridine, CZ 101-02-0 P(OPh)<sub>3</sub>  
CON 3 hours, 70 deg C

STAGE(2)

RCT DS 122-80-5  
CON 1 hour, 55 deg C

PRO DT 944915-41-7

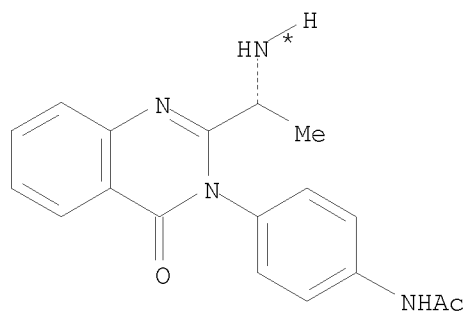
RX(73) OF 342 ...DT ==> EO...



DT

(73)  $\longrightarrow$

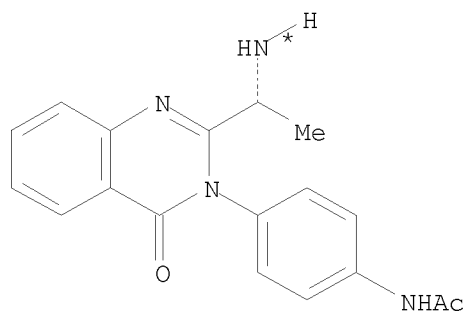
10/ 562,112



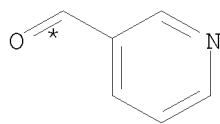
EO  
YIELD 90%

RX(73)      RCT    DT 944915-41-7  
              RGT    ED 76-05-1 F3CCO2H  
              PRO    EO 944915-56-4  
              SOL    75-09-2 CH2Cl2  
              CON    2 hours, room temperature

RX(98) OF 342      ...EO + FC ==> BV...

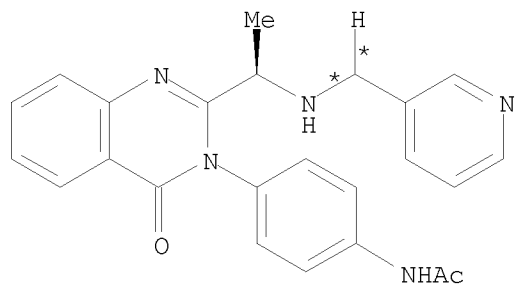


EO



FC

(98)  
→

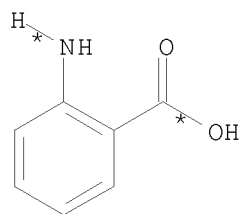


BV  
YIELD 80%

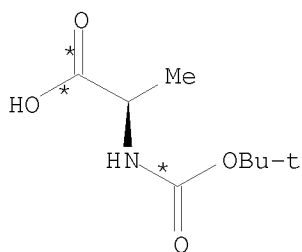
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RX(98) RCT EO 944915-56-4, FC 500-22-1  
RGT O 56553-60-7 Na.(AcO)3BH  
PRO BV 944915-81-5  
SOL 107-06-2 ClCH2CH2Cl  
CON 2 hours, room temperature

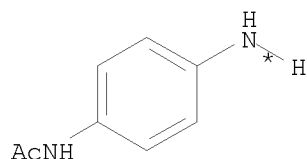
RX(137) OF 342 COMPOSED OF RX(57), RX(73)  
RX(137) CR + CQ + DS ==> EO



CR

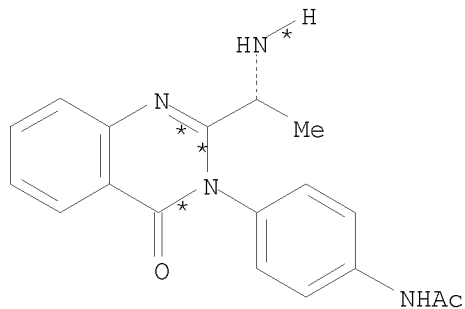


CQ



DS

2  
STEPS  
=>



EO  
YIELD 90%

RX(57) RCT CR 118-92-3, CQ 7764-95-6

STAGE(1)

RGT U 110-86-1 Pyridine, CZ 101-02-0 P(OPh)3  
CON 3 hours, 70 deg C

STAGE(2)

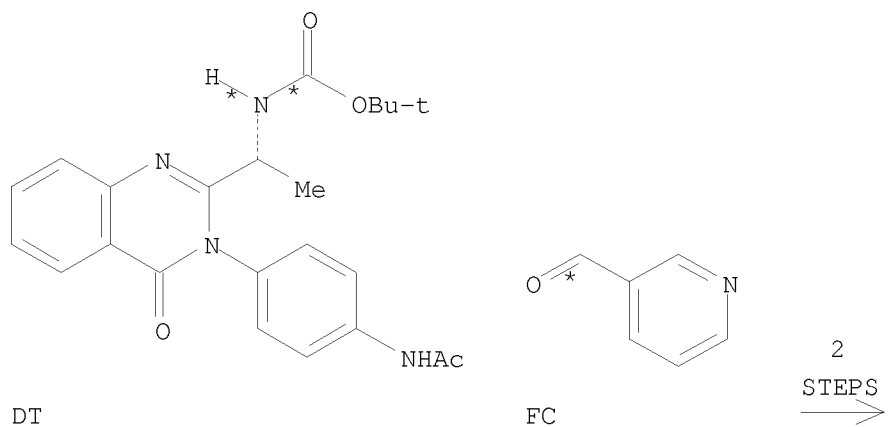
RCT DS 122-80-5  
CON 1 hour, 55 deg C

PRO DT 944915-41-7

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RX(73)     RCT   DT 944915-41-7  
             RGT   ED 76-05-1 F3CCO2H  
             PRO   EO 944915-56-4  
             SOL   75-09-2 CH2Cl2  
             CON   2 hours, room temperature

RX(163) OF 342 COMPOSED OF RX(73), RX(98)  
RX(163)   DT   +   FC   ==>   BV



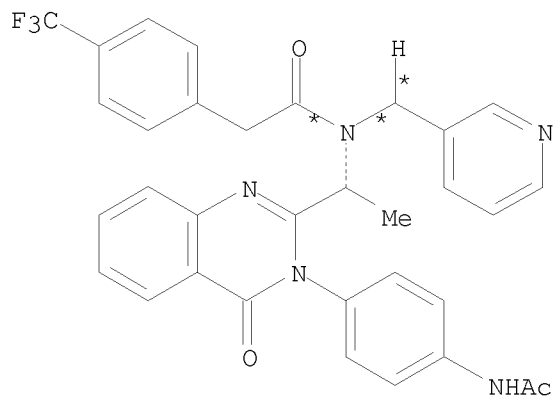
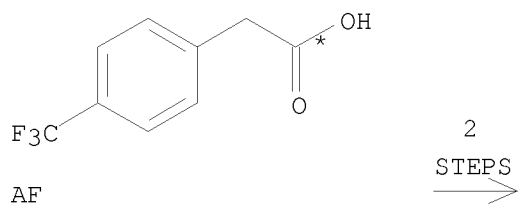
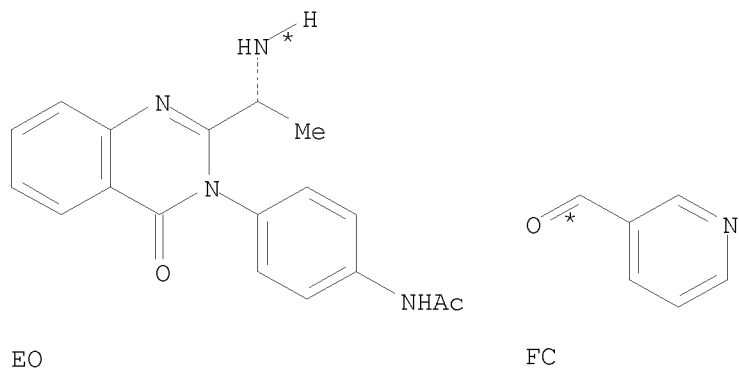
BV  
YIELD 80%

RX(73)     RCT   DT 944915-41-7  
             RGT   ED 76-05-1 F3CCO2H  
             PRO   EO 944915-56-4  
             SOL   75-09-2 CH2Cl2  
             CON   2 hours, room temperature

RX(98)     RCT   EO 944915-56-4, FC 500-22-1  
             RGT   O 56553-60-7 Na.(AcO)3BH  
             PRO   BV 944915-81-5  
             SOL   107-06-2 ClCH2CH2Cl  
             CON   2 hours, room temperature

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RX(202) OF 342 COMPOSED OF RX(98), RX(34)  
RX(202) EO + FC + AF ==> BW



BW  
YIELD 90%

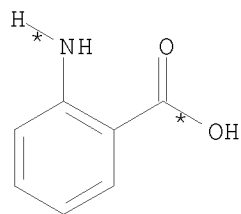
RX(98) RCT EO 944915-56-4, FC 500-22-1  
RGT O 56553-60-7 Na.(AcO)3BH  
PRO BV 944915-81-5  
SOL 107-06-2 ClCH2CH2Cl  
CON 2 hours, room temperature

RX(34) RCT BV 944915-81-5, AF 32857-62-8  
RGT D 2592-95-2 1-Benzotriazolol, E 25952-53-8 EDAP

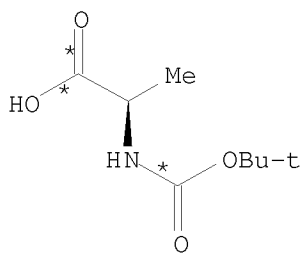
10/ 562,112

PRO BW 944915-21-3  
SOL 68-12-2 DMF  
CON 1 hour, room temperature

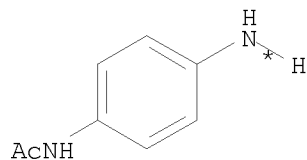
RX(246) OF 342 COMPOSED OF RX(57), RX(73), RX(98)  
RX(246) CR + CQ + DS + FC ==> BV



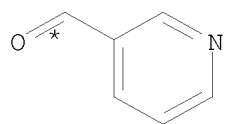
CR



CQ

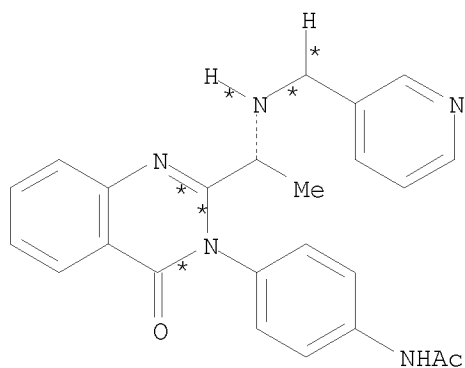


DS



FC

3  
STEPS  
→



BV  
YIELD 80%

RX(57) RCT CR 118-92-3, CQ 7764-95-6

STAGE(1)

RGT U 110-86-1 Pyridine, CZ 101-02-0 P(OPh)<sub>3</sub>  
CON 3 hours, 70 deg C

STAGE(2)

RCT DS 122-80-5  
CON 1 hour, 55 deg C



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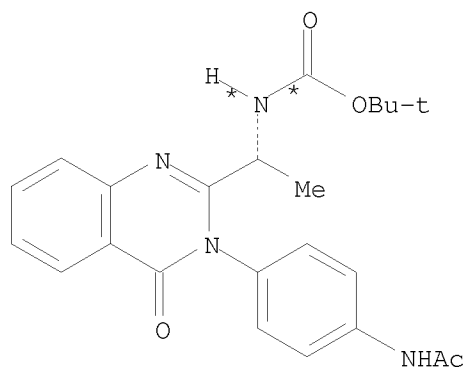
PRO DT 944915-41-7

RX(73) RCT DT 944915-41-7  
RGT ED 76-05-1 F3CCO2H  
PRO EO 944915-56-4  
SOL 75-09-2 CH2Cl2  
CON 2 hours, room temperature

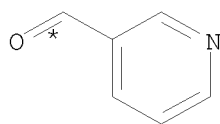
RX(98) RCT EO 944915-56-4, FC 500-22-1  
RGT O 56553-60-7 Na.(AcO)3BH  
PRO BV 944915-81-5  
SOL 107-06-2 ClCH2CH2Cl  
CON 2 hours, room temperature

RX(321) OF 342 COMPOSED OF RX(73), RX(98), RX(34)

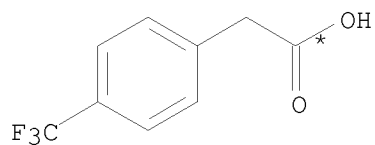
RX(321) DT + FC + AF ==> BW



DT



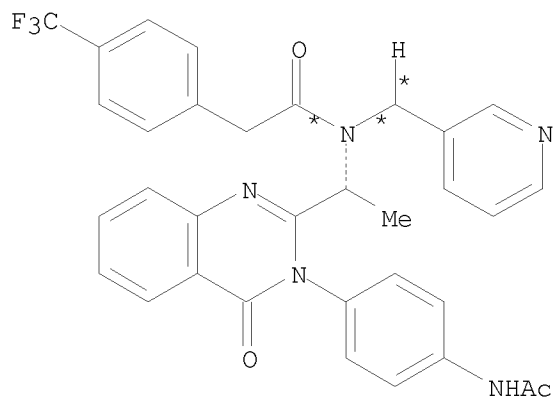
FC



AF

3  
STEPS  
→

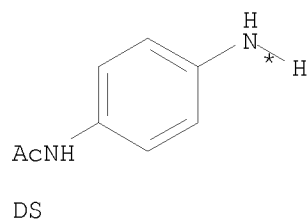
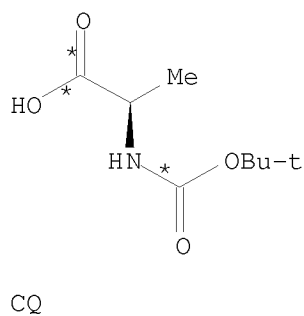
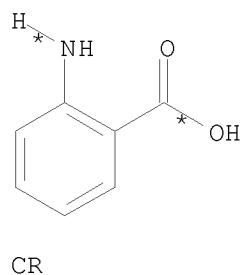
10/ 562,112



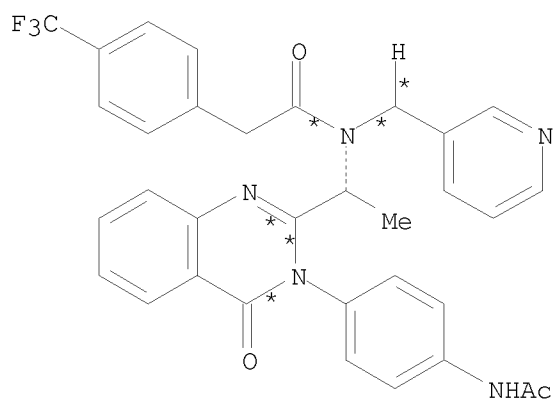
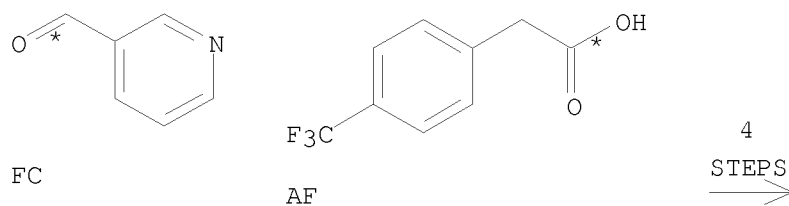
BW  
YIELD 90%

RX(73)	RCT	DT 944915-41-7
	RGT	ED 76-05-1 F3CCO2H
	PRO	EO 944915-56-4
	SOL	75-09-2 CH2Cl2
	CON	2 hours, room temperature
RX(98)	RCT	EO 944915-56-4, FC 500-22-1
	RGT	O 56553-60-7 Na.(AcO)3BH
	PRO	BV 944915-81-5
	SOL	107-06-2 ClCH2CH2Cl
	CON	2 hours, room temperature
RX(34)	RCT	BV 944915-81-5, AF 32857-62-8
	RGT	D 2592-95-2 1-Benzotriazolol, E 25952-53-8 EDAP
	PRO	BW 944915-21-3
	SOL	68-12-2 DMF
	CON	1 hour, room temperature

RX(322) OF 342 COMPOSED OF RX(57), RX(73), RX(98), RX(34)  
RX(322) CR + CQ + DS + FC + AF ==> BW



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BW  
YIELD 90%

RX(57) RCT CR 118-92-3, CQ 7764-95-6

STAGE(1)

RGT U 110-86-1 Pyridine, CZ 101-02-0 P(OPh)<sub>3</sub>  
CON 3 hours, 70 deg C

STAGE(2)

RCT DS 122-80-5  
CON 1 hour, 55 deg C

PRO DT 944915-41-7

RX(73) RCT DT 944915-41-7  
RGT ED 76-05-1 F<sub>3</sub>CCO<sub>2</sub>H  
PRO EO 944915-56-4  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 2 hours, room temperature

RX(98) RCT EO 944915-56-4, FC 500-22-1  
RGT O 56553-60-7 Na.(AcO)<sub>3</sub>BH  
PRO BV 944915-81-5  
SOL 107-06-2 ClCH<sub>2</sub>CH<sub>2</sub>Cl  
CON 2 hours, room temperature

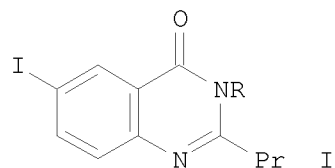
RX(34) RCT BV 944915-81-5, AF 32857-62-8  
RGT D 2592-95-2 1-Benzotriazolol, E 25952-53-8 EDAP  
PRO BW 944915-21-3  
SOL 68-12-2 DMF

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CON 1 hour, room temperature

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

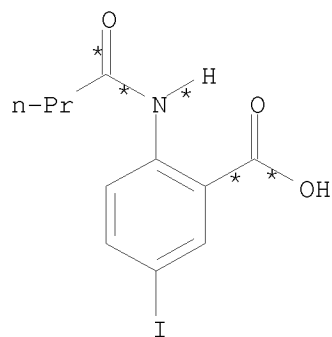
L3 ANSWER 19 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 147:211821 CASREACT  
TITLE: Synthesis of some new 4-(3H)-quinazoline analogs as potential antioxidant agents  
AUTHOR(S): Al-Omar, M. A.; El-Azab, Adel E.; El-Obeid, H. A.; Abdel Hamide, S. G.  
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, Riyadh, 11451, Saudi Arabia  
SOURCE: Journal of Saudi Chemical Society (2006), 10(1), 113-128  
CODEN: JSCSFO; ISSN: 1319-6103  
PUBLISHER: Saudi Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



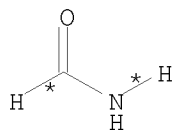
AB A new series of derivs. of 6-iodo-2-propyl-4(3H)-quinazolinone [I, R = H] and its fused heterocyclic analogs were prepared and screened for their antioxidant activity. I [R = H, NHCONH<sub>2</sub>, OH, phthalimido, NH<sub>2</sub>, O<sub>2</sub>CCH<sub>2</sub>Cl, OCH<sub>2</sub>CONH<sub>2</sub>] inhibit aldehyde oxidase exclusively by more than 98 %. This type of inhibition was found to be competitive with K<sub>i</sub> value ranging from 50-400 μM with respect to aldehyde oxidase.

RX(32) OF 118 COMPOSED OF RX(2), RX(4)  
RX(32) C + J ==> K

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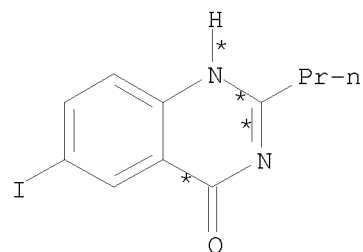


C



J

2  
STEPS  
→



K

YIELD 70%

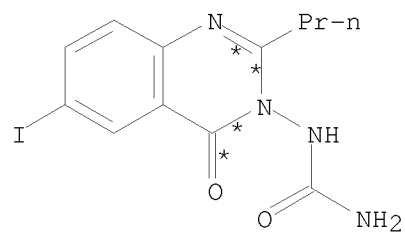
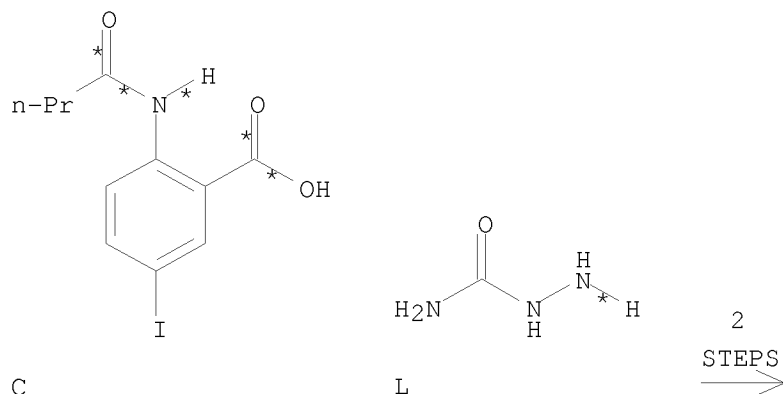
RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(4) RCT E 944830-81-3, J 75-12-7  
PRO K 145863-89-4  
SOL 75-12-7 Formamide  
CON 2 hours, reflux

RX(33) OF 118 COMPOSED OF RX(2), RX(5)

RX(33) C + L ==> M

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YIELD 85%

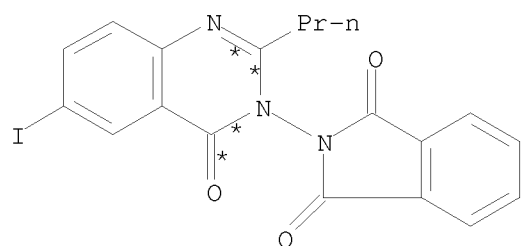
RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac2O
	CON	4 hours, reflux
RX(5)	RCT	E 944830-81-3, L 57-56-7
	PRO	M 944830-83-5
	SOL	110-86-1 Pyridine
	CON	6 hours, reflux

RX(34) OF 118 COMPOSED OF RX(2), RX(7)

RX(34) C ==> Q



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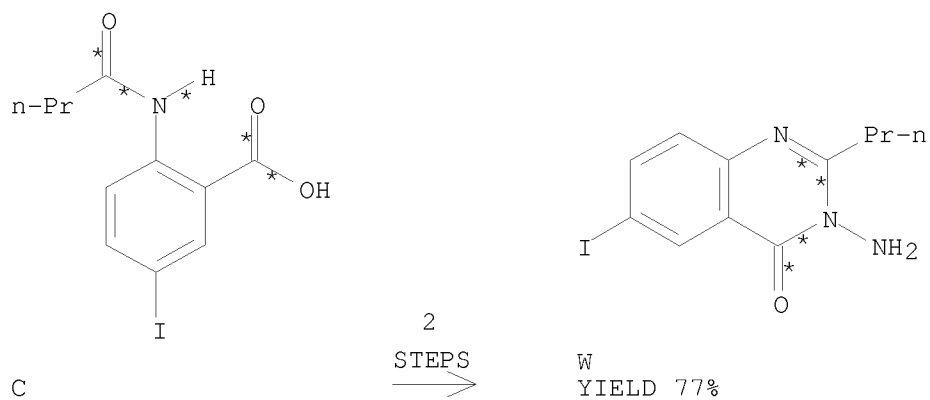


V  
YIELD 72%

RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(9) RCT E 944830-81-3, U 1875-48-5  
PRO V 944830-87-9  
SOL 110-86-1 Pyridine  
CON 6 - 12 hours, reflux

RX(37) OF 118 COMPOSED OF RX(2), RX(10)  
RX(37) C ==> W



RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

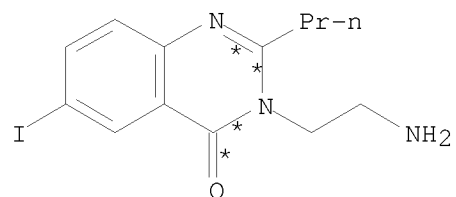
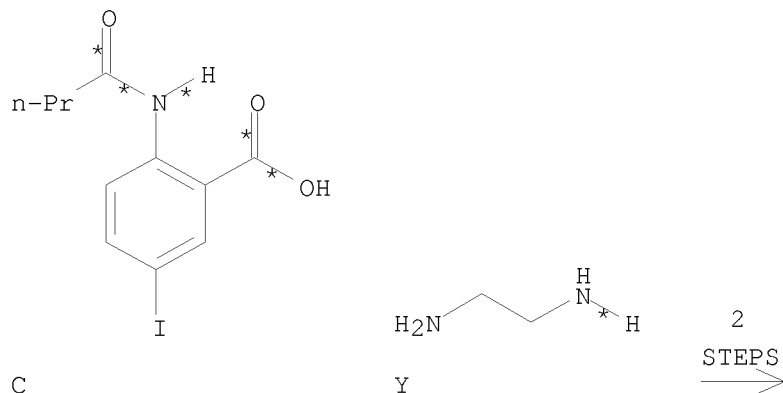
RX(10) RCT E 944830-81-3  
RGT X 7803-57-8 N2H4-H2O  
PRO W 944830-88-0  
CON 1 hour, heated

RX(38) OF 118 COMPOSED OF RX(2), RX(11)



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RX(38)      C   +   Y   ==>   Z



Z  
YIELD 45%

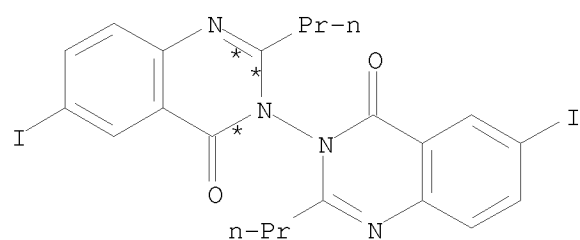
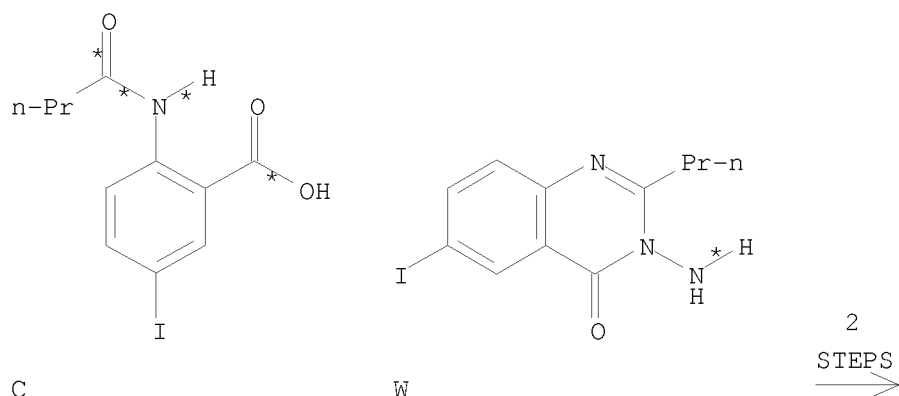
RX(2)      RCT   C 73721-77-4  
             PRO   E 944830-81-3  
             SOL   108-24-7 Ac2O  
             CON   4 hours, reflux

RX(11)      RCT   E 944830-81-3, Y 107-15-3  
             PRO   Z 944830-89-1  
             SOL   64-17-5 EtOH  
             CON   2 hours, reflux

RX(39) OF 118 COMPOSED OF RX(2), RX(12)

RX(39)      C   +   W   ==>   AB

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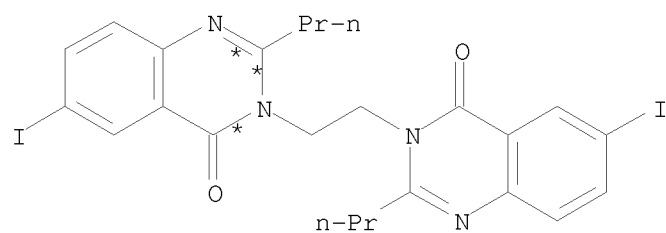
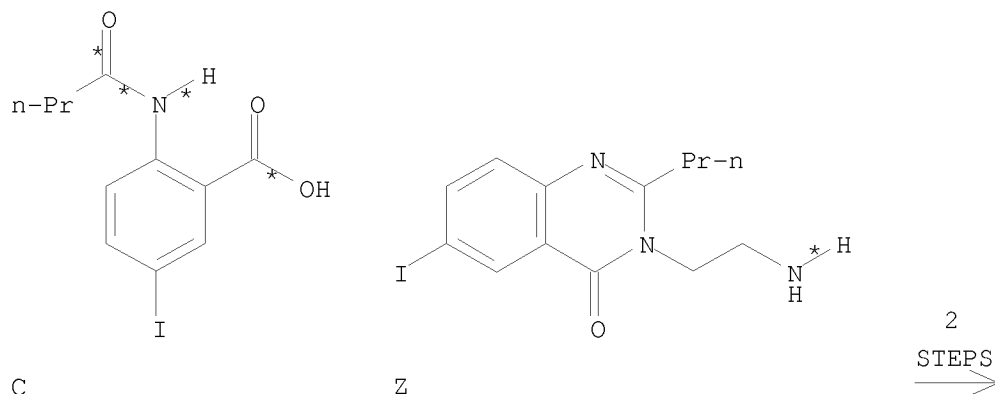
AB  
YIELD 63%

RX(2)      RCT    C 73721-77-4  
              PRO    E 944830-81-3  
              SOL    108-24-7 Ac2O  
              CON    4 hours, reflux

RX(12)     RCT    E 944830-81-3, W 944830-88-0  
              RGT    O 127-09-3 AcONa  
              PRO    AB 944830-90-4  
              SOL    64-19-7 AcOH  
              CON    18 hours, reflux

RX(40) OF 118 COMPOSED OF RX(2), RX(13)  
 RX(40)      C    +    Z    ==>    AC

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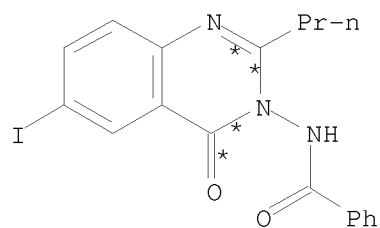
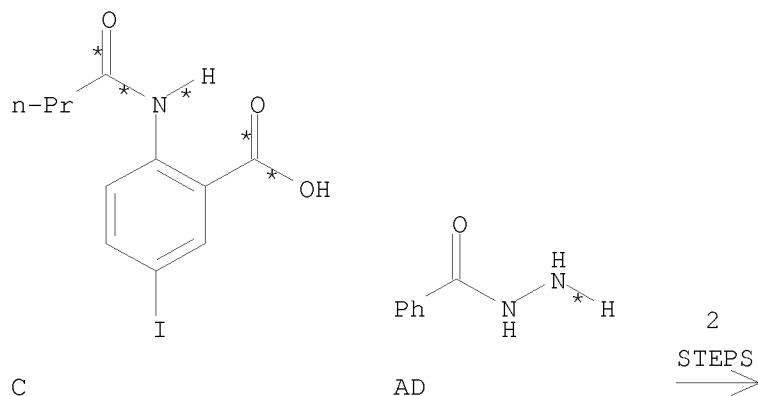
AC  
YIELD 56%

RX(2)      RCT    C 73721-77-4  
              PRO    E 944830-81-3  
              SOL    108-24-7 Ac2O  
              CON    4 hours, reflux

RX(13)     RCT    E 944830-81-3, Z 944830-89-1  
              RGT    O 127-09-3 AcONa  
              PRO    AC 944830-91-5  
              SOL    64-19-7 AcOH  
              CON    18 hours, reflux

RX(41) OF 118 COMPOSED OF RX(2), RX(14)  
 RX(41)      C    +    AD    ==>    AE

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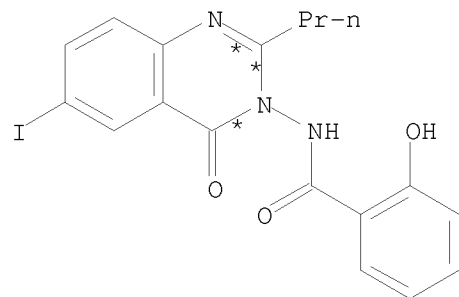
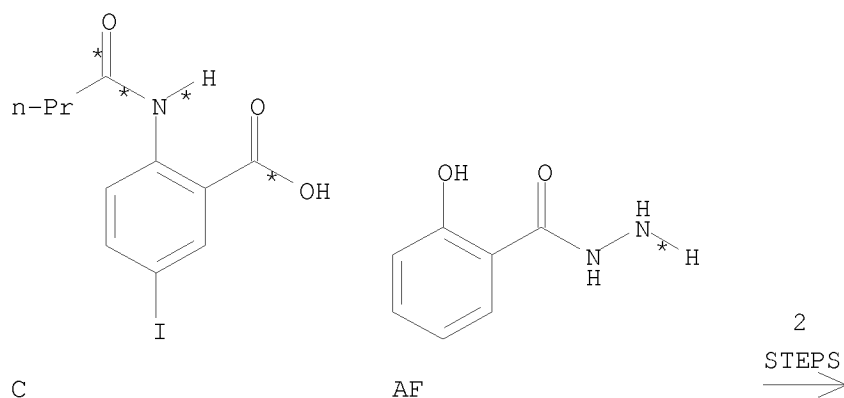
AE  
YIELD 73%

RX(2)      RCT    C 73721-77-4  
              PRO    E 944830-81-3  
              SOL    108-24-7 Ac2O  
              CON    4 hours, reflux

RX(14)     RCT    E 944830-81-3, AD 613-94-5  
              PRO    AE 944830-93-7  
              SOL    110-86-1 Pyridine  
              CON    10 hours, reflux  
              NTE    alternative preparation shown

RX(42) OF 118 COMPOSED OF RX(2), RX(15)  
 RX(42)      C    +    AF    ==>    AG

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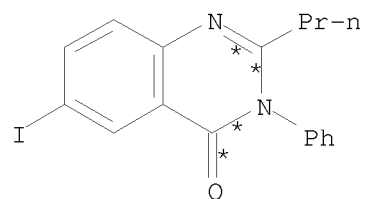
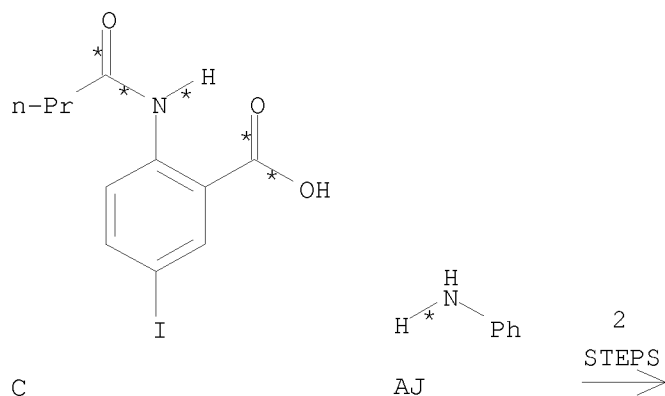
AG  
YIELD 71%

RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(15) RCT E 944830-81-3, AF 936-02-7  
PRO AG 944830-94-8  
SOL 110-86-1 Pyridine  
CON 10 hours, reflux

RX(43) OF 118 COMPOSED OF RX(2), RX(17)  
RX(43) C + AJ ==> AK

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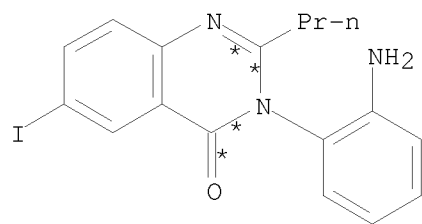
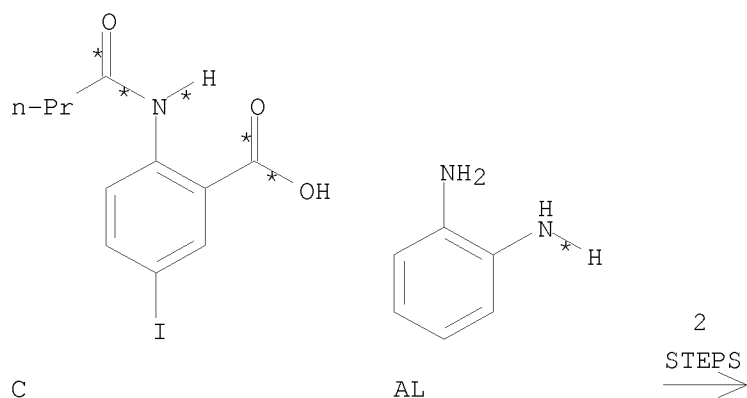
AK  
YIELD 76%

RX(2)      RCT   C 73721-77-4  
             PRO   E 944830-81-3  
             SOL   108-24-7 Ac2O  
             CON   4 hours, reflux

RX(17)     RCT   E 944830-81-3, AJ 62-53-3  
             PRO   AK 944830-96-0  
             SOL   110-86-1 Pyridine  
             CON   6 - 12 hours, reflux

RX(44) OF 118 COMPOSED OF RX(2), RX(18)  
RX(44)      C   +   AL   ==>   AM

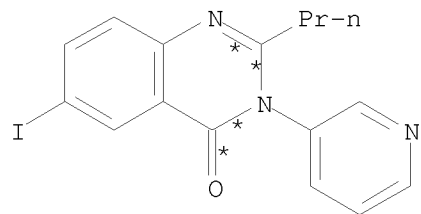
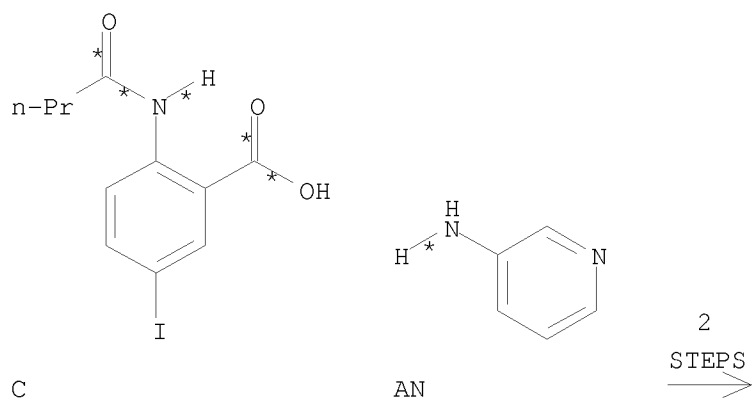
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AM  
YIELD 80%

RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac2O
	CON	4 hours, reflux
RX(18)	RCT	E 944830-81-3, AL 95-54-5
	PRO	AM 944830-97-1
	SOL	110-86-1 Pyridine
	CON	6 - 12 hours, reflux
RX(45) OF 118 COMPOSED OF RX(2), RX(19)		
RX(45)	C + AN	==> AO

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AO  
YIELD 83%

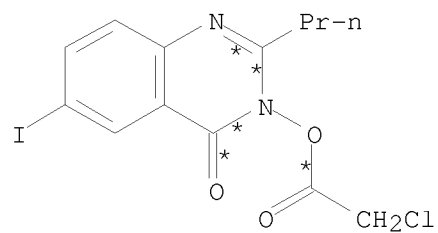
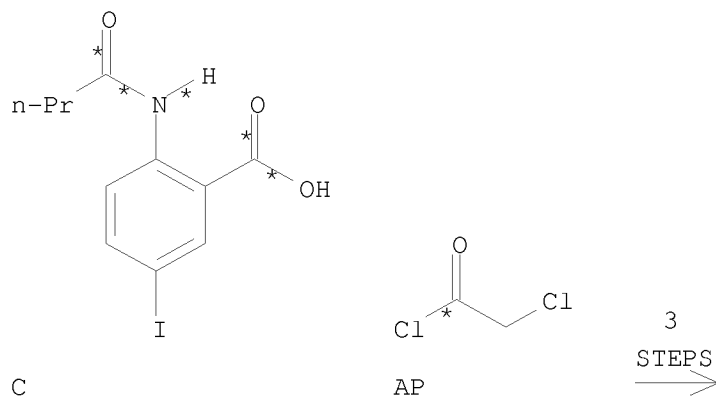
RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(19) RCT E 944830-81-3, AN 462-08-8  
PRO AO 944830-98-2  
SOL 110-86-1 Pyridine  
CON 6 - 12 hours, reflux

RX(76) OF 118 COMPOSED OF RX(2), RX(7), RX(20)  
RX(76) C + AP ==> AQ



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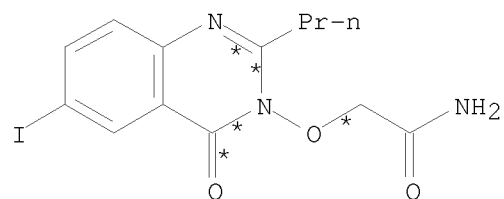
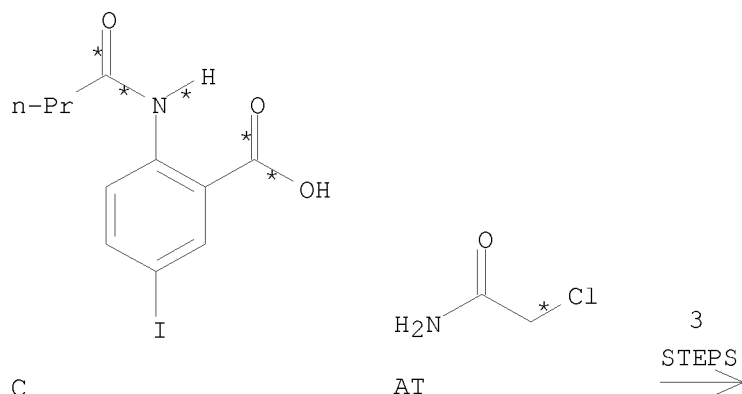


AQ  
YIELD 80%

RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac2O
	CON	4 hours, reflux
RX(7)	RCT	E 944830-81-3
	RGT	R 5470-11-1 H2NOH-HCl
	PRO	Q 944830-85-7
	SOL	110-86-1 Pyridine
	CON	6 - 12 hours, reflux
RX(20)	RCT	Q 944830-85-7, AP 79-04-9
	PRO	AQ 944830-99-3
	SOL	68-12-2 DMF
	CON	6 hours, reflux

RX(77) OF 118 COMPOSED OF RX(2), RX(7), RX(22)  
 RX(77) C + AT ==> AU

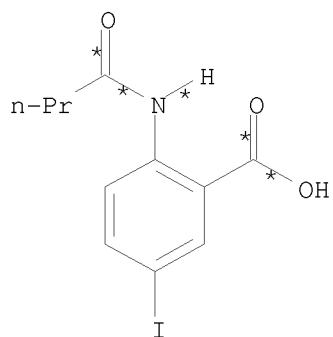
10/ 562,112



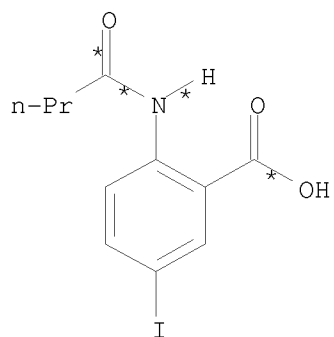
AU  
YIELD 88%

RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac <sub>2</sub> O
	CON	4 hours, reflux
RX(7)	RCT	E 944830-81-3
	RGT	R 5470-11-1 H <sub>2</sub> NOH-HCl
	PRO	Q 944830-85-7
	SOL	110-86-1 Pyridine
	CON	6 - 12 hours, reflux
RX(22)	RCT	Q 944830-85-7, AT 79-07-2
	PRO	AU 944831-01-0
	SOL	68-12-2 DMF
	CON	6 hours, reflux

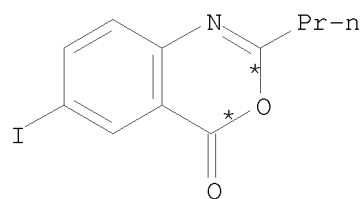
RX(78) OF 118 COMPOSED OF RX(2), RX(10), RX(12)  
RX(78) 2 C + E ==> AB



C

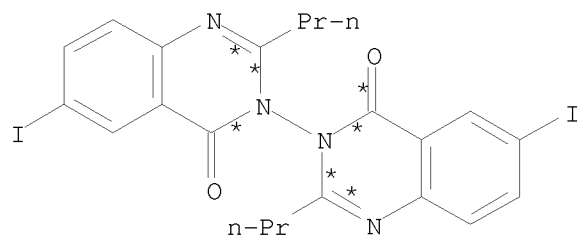


C



E

3  
STEPS  
→



AB  
YIELD 63%

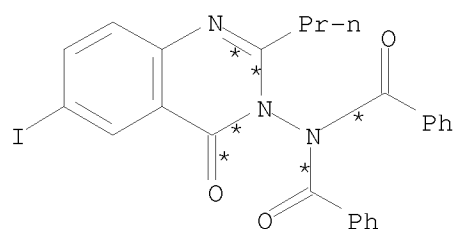
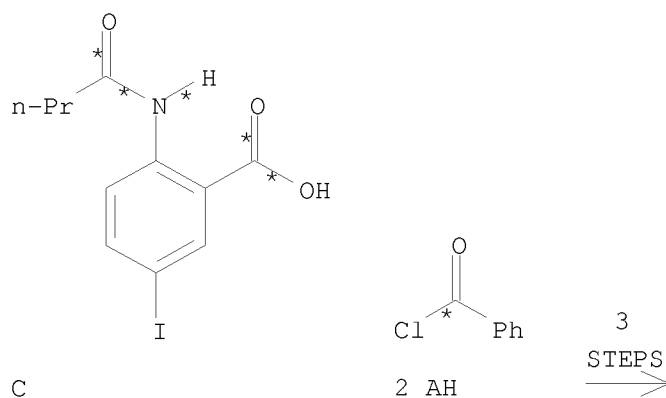
RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac2O
	CON	4 hours, reflux
RX(10)	RCT	E 944830-81-3
	RGT	X 7803-57-8 N2H4-H2O
	PRO	W 944830-88-0
	CON	1 hour, heated
RX(12)	RCT	E 944830-81-3, W 944830-88-0
	RGT	O 127-09-3 AcONa
	PRO	AB 944830-90-4
	SOL	64-19-7 AcOH

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CON 18 hours, reflux

RX(79) OF 118 COMPOSED OF RX(2), RX(10), RX(16)

RX(79) C + 2 AH ==> AI



AI  
YIELD 81%

RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

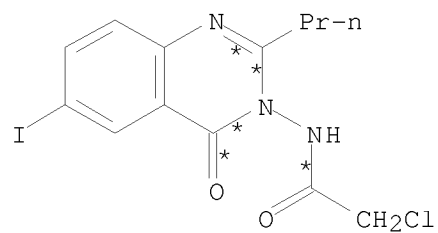
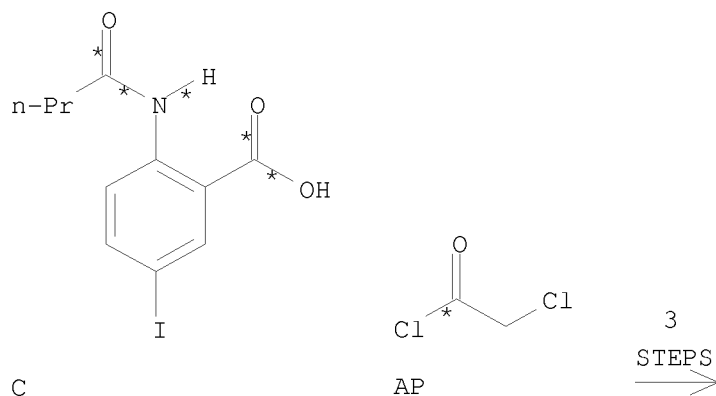
RX(10) RCT E 944830-81-3  
RGT X 7803-57-8 N2H4-H2O  
PRO W 944830-88-0  
CON 1 hour, heated

RX(16) RCT W 944830-88-0, AH 98-88-4  
PRO AI 944830-95-9  
SOL 110-86-1 Pyridine  
CON 7 hours, reflux

RX(80) OF 118 COMPOSED OF RX(2), RX(10), RX(21)

RX(80) C + AP ==> AS

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AS  
YIELD 71%

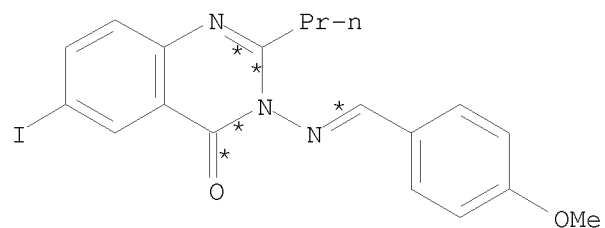
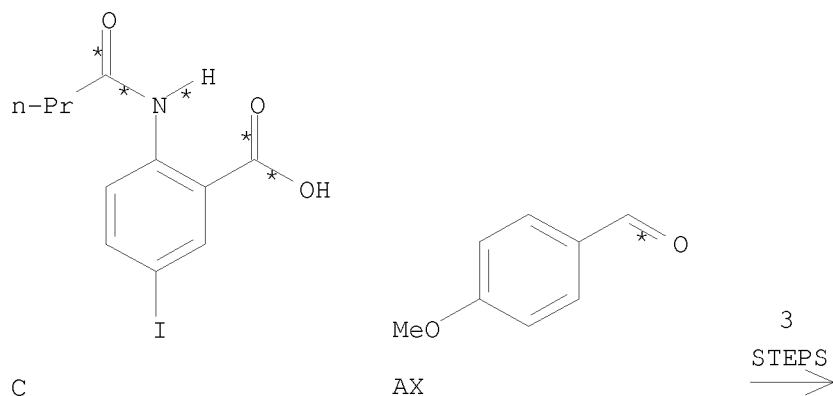
RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(10) RCT E 944830-81-3  
RGT X 7803-57-8 N2H4-H2O  
PRO W 944830-88-0  
CON 1 hour, heated

RX(21) RCT W 944830-88-0, AP 79-04-9  
PRO AS 944831-00-9  
SOL 68-12-2 DMF  
CON 5 hours, room temperature

RX(81) OF 118 COMPOSED OF RX(2), RX(10), RX(24)  
RX(81) C + AX ==> AY

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AY  
YIELD 79%

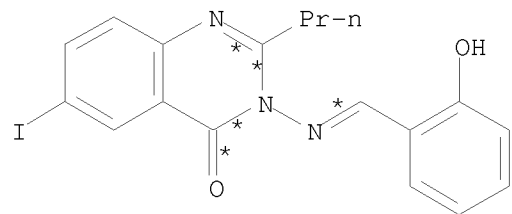
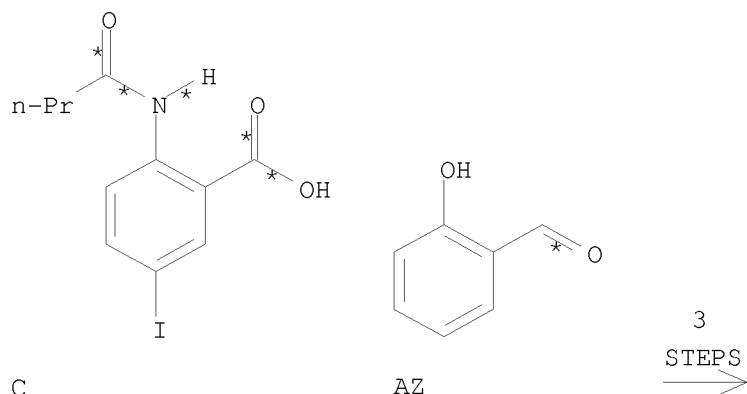
RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(10) RCT E 944830-81-3  
RGT X 7803-57-8 N2H4-H2O  
PRO W 944830-88-0  
CON 1 hour, heated

RX(24) RCT W 944830-88-0, AX 123-11-5  
PRO AY 944831-03-2  
SOL 64-19-7 AcOH  
CON 9 hours, reflux

RX(82) OF 118 COMPOSED OF RX(2), RX(10), RX(25)  
RX(82) C + AZ ==> BA

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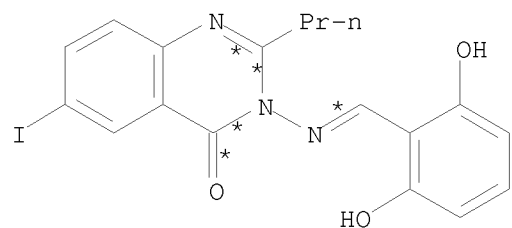
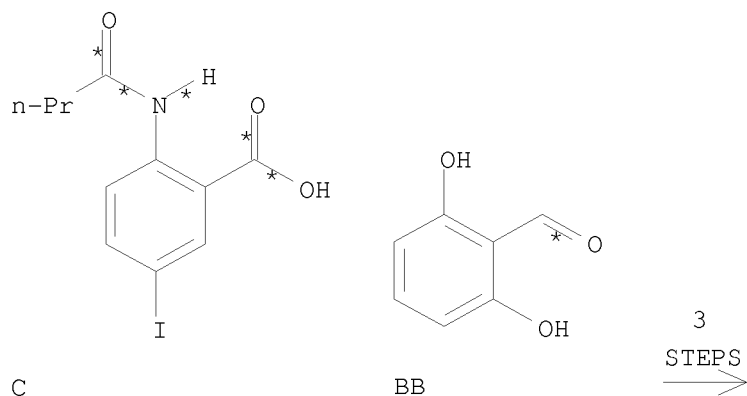


YIELD 83%

RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac2O
	CON	4 hours, reflux
RX(10)	RCT	E 944830-81-3
	RGT	X 7803-57-8 N2H4-H2O
	PRO	W 944830-88-0
	CON	1 hour, heated
RX(25)	RCT	W 944830-88-0, AZ 90-02-8
	PRO	BA 944831-04-3
	SOL	64-19-7 AcOH
	CON	9 hours, reflux

RX(83) OF 118 COMPOSED OF RX(2), RX(10), RX(26)  
 RX(83) C + BB ==> BC

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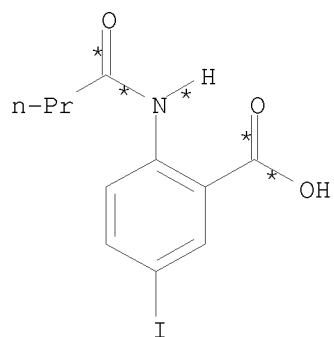
BC  
YIELD 70%

RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac2O
	CON	4 hours, reflux
RX(10)	RCT	E 944830-81-3
	RGT	X 7803-57-8 N2H4-H2O
	PRO	W 944830-88-0
	CON	1 hour, heated
RX(26)	RCT	W 944830-88-0, BB 387-46-2
	PRO	BC 944831-05-4
	SOL	64-19-7 AcOH
	CON	9 hours, reflux

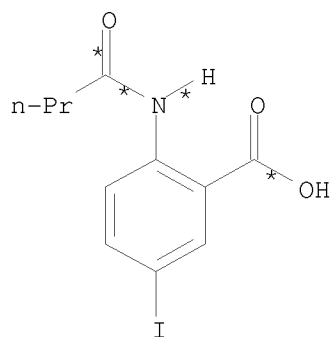
RX(84) OF 118 COMPOSED OF RX(2), RX(11), RX(13)  
RX(84) 2 C + Y + E ==> AC



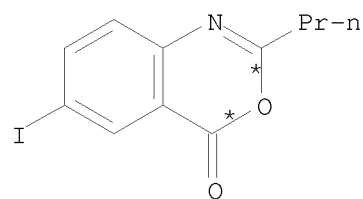
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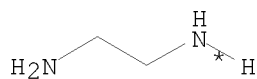
C



C

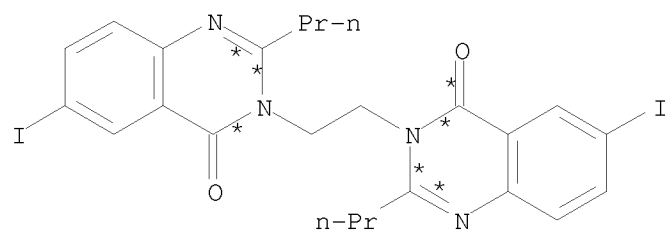


E



Y

3  
STEPS  
→



AC  
YIELD 56%

RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(11) RCT E 944830-81-3, Y 107-15-3  
PRO Z 944830-89-1  
SOL 64-17-5 EtOH  
CON 2 hours, reflux

RX(13) RCT E 944830-81-3, Z 944830-89-1  
RGT O 127-09-3 AcONa  
PRO AC 944830-91-5  
SOL 64-19-7 AcOH

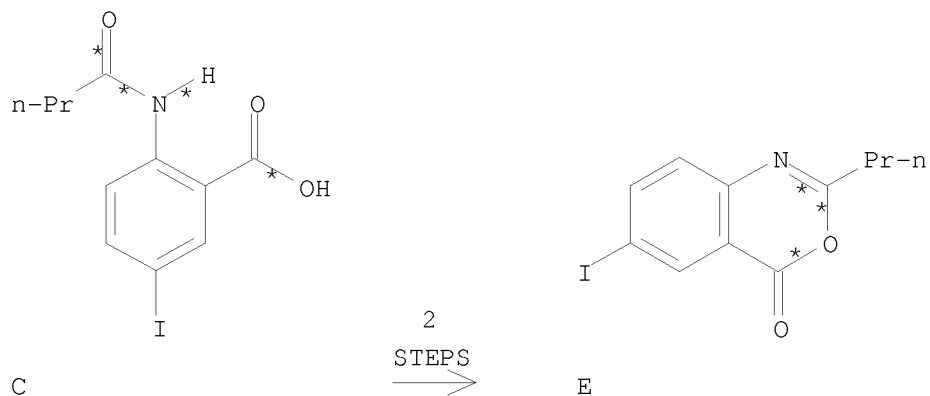
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CON 18 hours, reflux

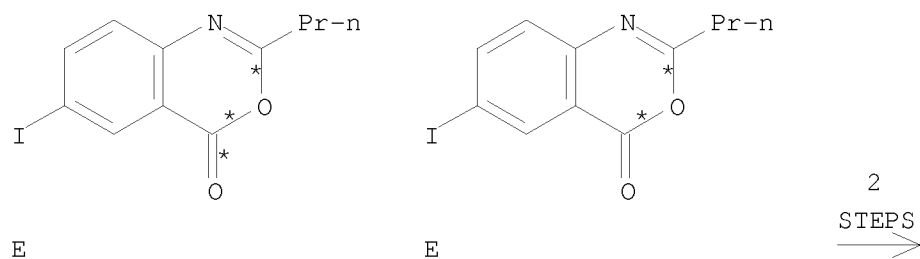
RX(97) OF 118 COMPOSED OF REACTION SEQUENCE RX(2), RX(12)  
AND REACTION SEQUENCE RX(10), RX(12)

... C ==> E...

...2 E ==> AB



START NEXT REACTION SEQUENCE



AB  
YIELD 63%

RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(10) RCT E 944830-81-3  
RGT X 7803-57-8 N2H4-H2O

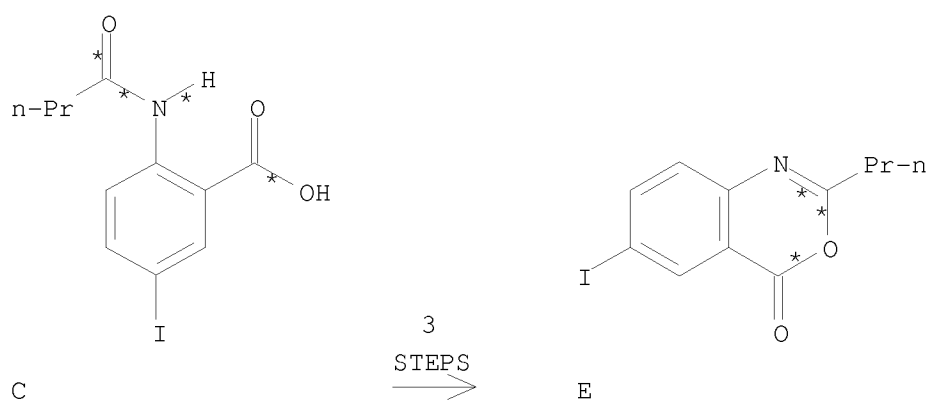
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PRO W 944830-88-0  
CON 1 hour, heated

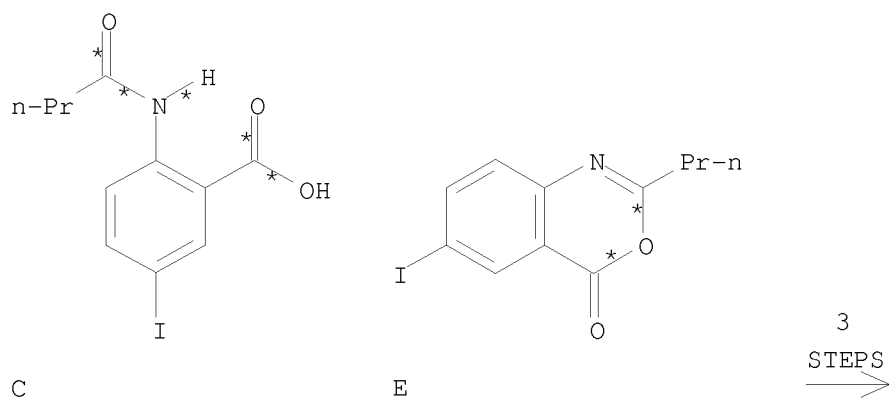
RX(12) RCT E 944830-81-3, W 944830-88-0  
RGT O 127-09-3 AcONa  
PRO AB 944830-90-4  
SOL 64-19-7 AcOH  
CON 18 hours, reflux

RX(101) OF 118 COMPOSED OF REACTION SEQUENCE RX(2), RX(12)  
AND REACTION SEQUENCE RX(2), RX(10), RX(12)

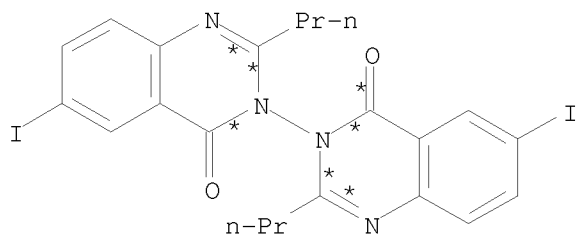
... C ==> E...  
... C + E ==> AB



START NEXT REACTION SEQUENCE



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AB  
YIELD 63%

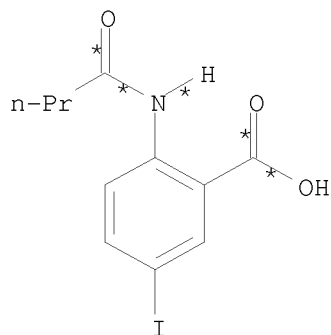
RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

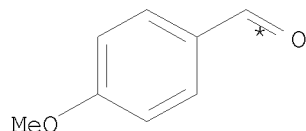
RX(10) RCT E 944830-81-3  
RGT X 7803-57-8 N2H4-H2O  
PRO W 944830-88-0  
CON 1 hour, heated

RX(12) RCT E 944830-81-3, W 944830-88-0  
RGT O 127-09-3 AcONa  
PRO AB 944830-90-4  
SOL 64-19-7 AcOH  
CON 18 hours, reflux

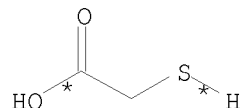
RX(102) OF 118 COMPOSED OF RX(2), RX(10), RX(24), RX(27)  
RX(102) C + AX + BD ==> BE



C



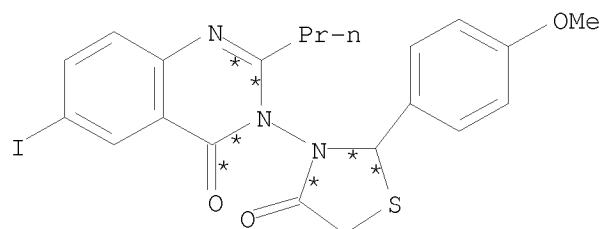
AX



BD

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4  
STEPS  
→



BE  
YIELD 60%

RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(10) RCT E 944830-81-3  
RGT X 7803-57-8 N2H4-H2O  
PRO W 944830-88-0  
CON 1 hour, heated

RX(24) RCT W 944830-88-0, AX 123-11-5  
PRO AY 944831-03-2  
SOL 64-19-7 AcOH  
CON 9 hours, reflux

RX(27) RCT AY 944831-03-2, BD 68-11-1

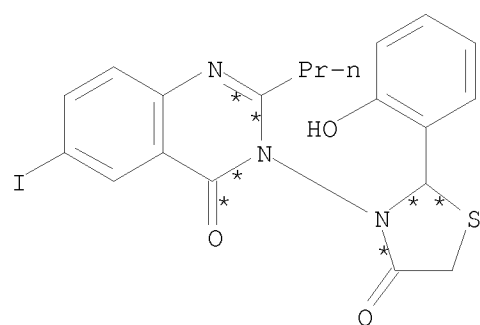
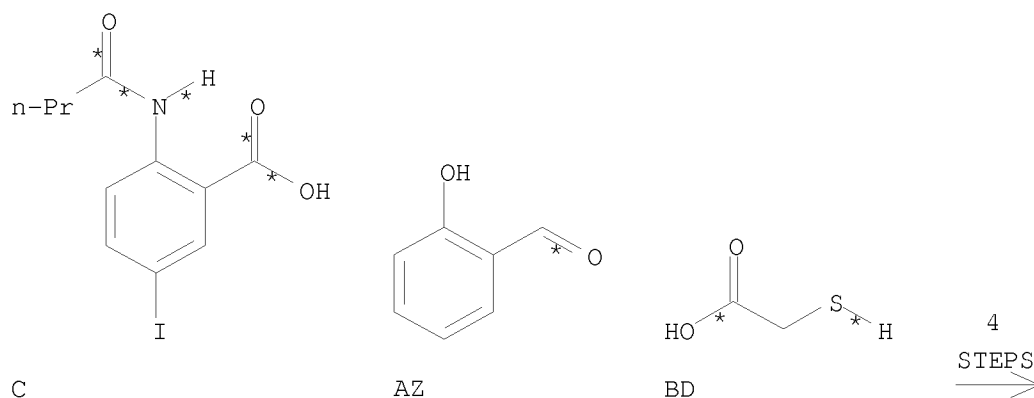
STAGE(1)  
SOL 71-43-2 Benzene  
CON 12 hours, reflux

STAGE(2)  
RGT BF 497-19-8 Na2CO3  
SOL 7732-18-5 Water  
CON neutralized

PRO BE 944831-06-5

RX(103) OF 118 COMPOSED OF RX(2), RX(10), RX(25), RX(28)  
RX(103) C + AZ + BD ==> BH

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BH  
YIELD 55%

RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac2O
	CON	4 hours, reflux
RX(10)	RCT	E 944830-81-3
	RGT	X 7803-57-8 N2H4-H2O
	PRO	W 944830-88-0
	CON	1 hour, heated
RX(25)	RCT	W 944830-88-0, AZ 90-02-8
	PRO	BA 944831-04-3
	SOL	64-19-7 AcOH
	CON	9 hours, reflux
RX(28)	RCT	BA 944831-04-3, BD 68-11-1
STAGE(1)		
	SOL	71-43-2 Benzene
	CON	12 hours, reflux
STAGE(2)		
	RGT	BF 497-19-8 Na2CO3
	SOL	7732-18-5 Water

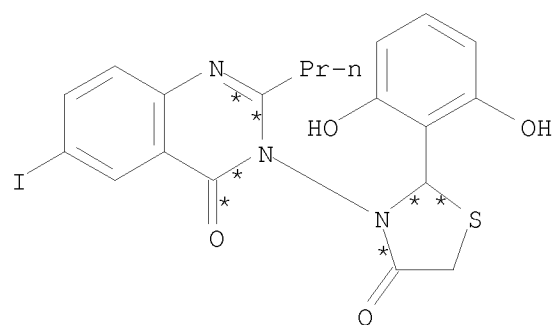
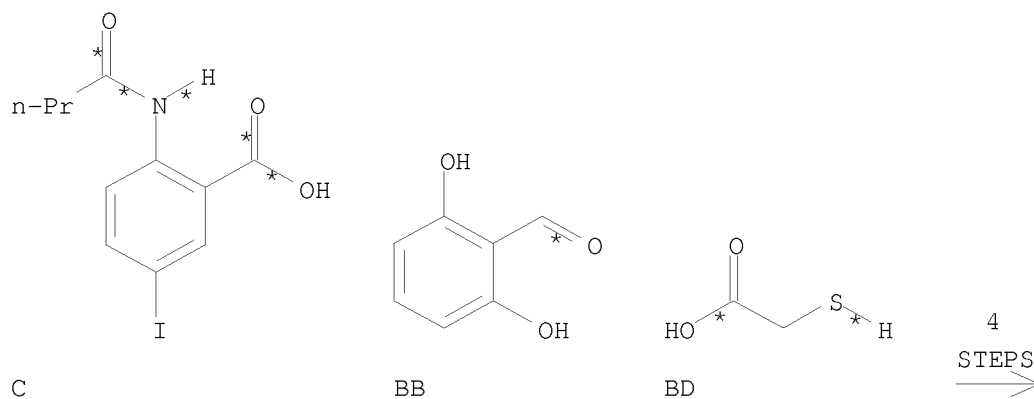
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CON neutralized

PRO BH 944831-07-6

RX(104) OF 118 COMPOSED OF RX(2), RX(10), RX(26), RX(29)

RX(104) C + BB + BD ==> BI



BI  
YIELD 51%

RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(10) RCT E 944830-81-3  
RGT X 7803-57-8 N2H4-H2O  
PRO W 944830-88-0  
CON 1 hour, heated

RX(26) RCT W 944830-88-0, BB 387-46-2  
PRO BC 944831-05-4  
SOL 64-19-7 AcOH  
CON 9 hours, reflux

RX(29) RCT BC 944831-05-4, BD 68-11-1

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STAGE(1)

SOL 71-43-2 Benzene  
CON 12 hours, reflux

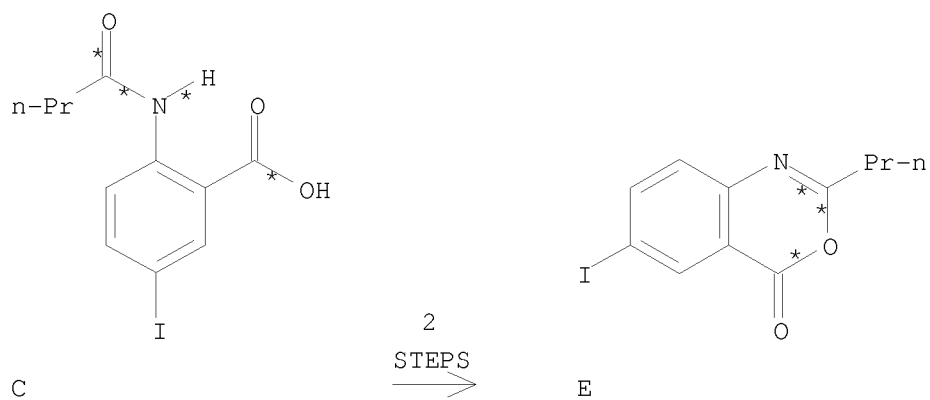
STAGE(2)

RGT BF 497-19-8 Na2CO3  
SOL 7732-18-5 Water  
CON neutralized

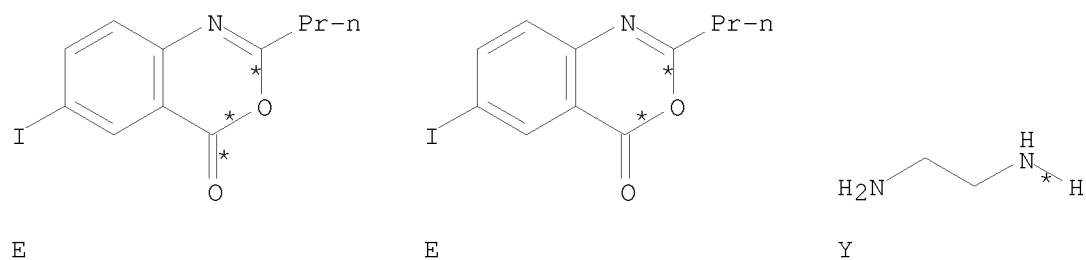
PRO BI 944831-08-7

RX(105) OF 118 COMPOSED OF REACTION SEQUENCE RX(2), RX(13)  
AND REACTION SEQUENCE RX(11), RX(13)

... C ==> E...  
...2 E + Y ==> AC

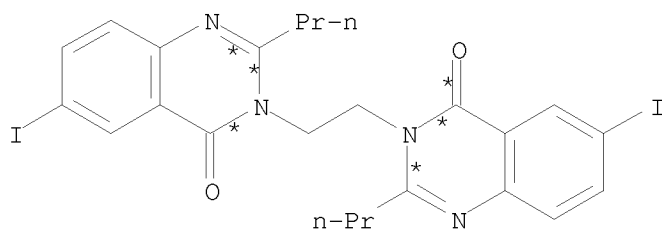


START NEXT REACTION SEQUENCE





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AC  
YIELD 56%

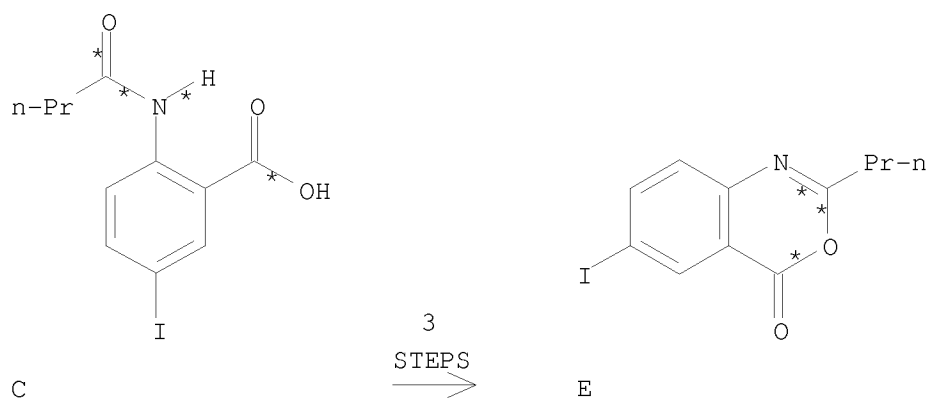
RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(11) RCT E 944830-81-3, Y 107-15-3  
PRO Z 944830-89-1  
SOL 64-17-5 EtOH  
CON 2 hours, reflux

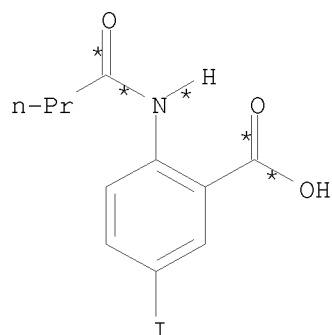
RX(13) RCT E 944830-81-3, Z 944830-89-1  
RGT O 127-09-3 AcONa  
PRO AC 944830-91-5  
SOL 64-19-7 AcOH  
CON 18 hours, reflux

RX(106) OF 118 COMPOSED OF REACTION SEQUENCE RX(2), RX(13)  
AND REACTION SEQUENCE RX(2), RX(11), RX(13)

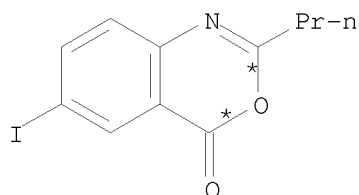
... C ==> E...  
... C + Y + E ==> AC



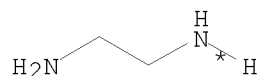
START NEXT REACTION SEQUENCE



C

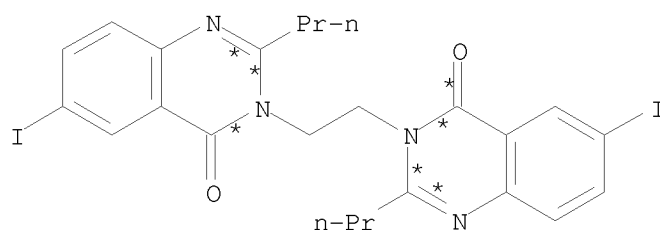


E



Y

3  
STEPS  
→



AC  
YIELD 56%

RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(11) RCT E 944830-81-3, Y 107-15-3  
PRO Z 944830-89-1  
SOL 64-17-5 EtOH  
CON 2 hours, reflux

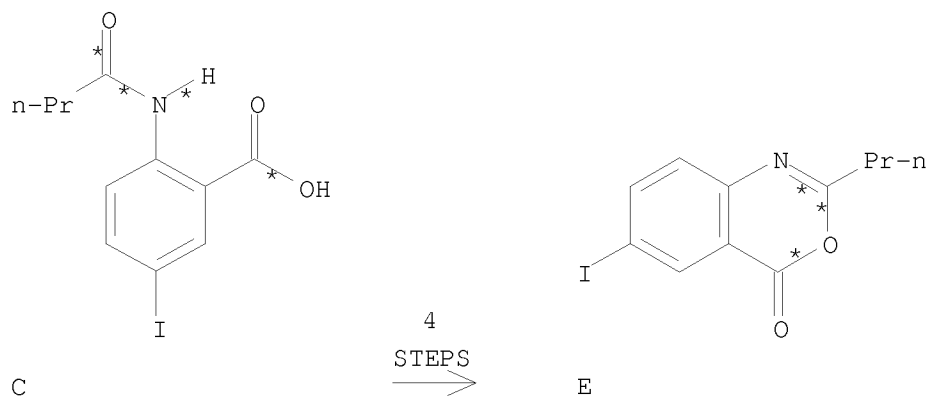
RX(13) RCT E 944830-81-3, Z 944830-89-1  
RGT O 127-09-3 AcONa  
PRO AC 944830-91-5  
SOL 64-19-7 AcOH  
CON 18 hours, reflux

RX(109) OF 118 COMPOSED OF REACTION SEQUENCE RX(2), RX(12)  
AND REACTION SEQUENCE RX(1), RX(2), RX(10), RX(12)

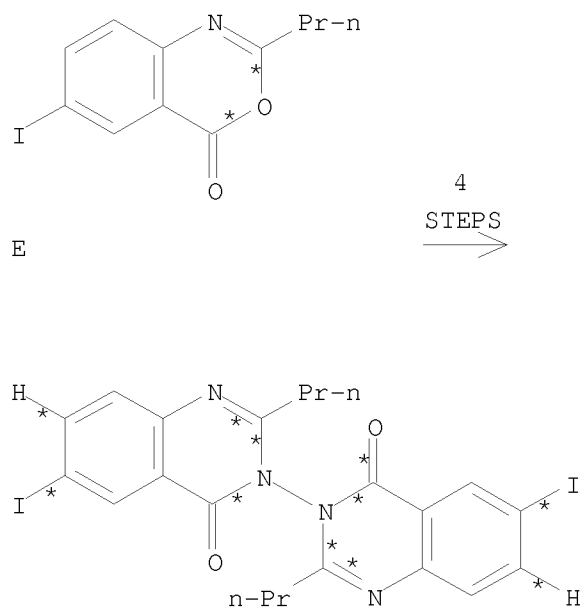
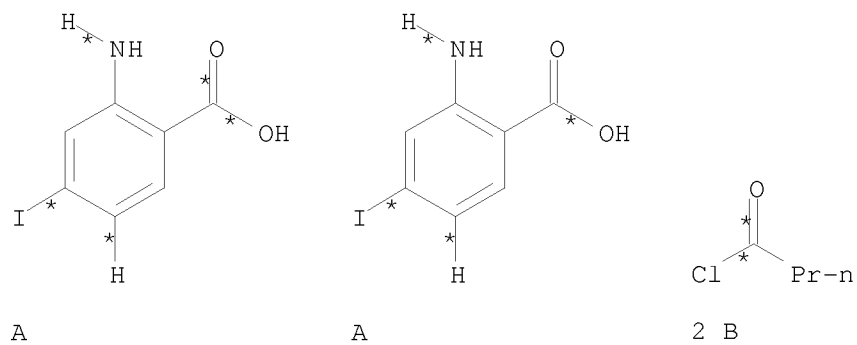
... C ==> E...

...2 A + 2 B + E ==> AB

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START NEXT REACTION SEQUENCE



YIELD 63%

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RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(1) RCT A 20776-54-9, B 141-75-3  
PRO C 73721-77-4  
SOL 110-86-1 Pyridine  
CON 2 hours, room temperature

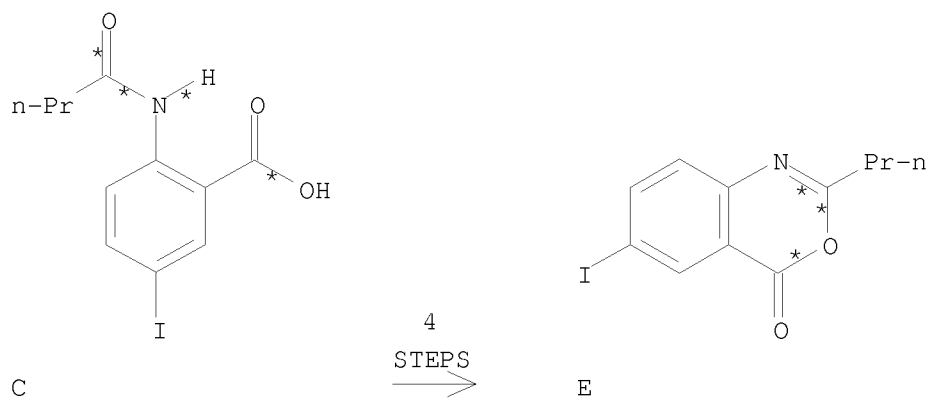
RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(10) RCT E 944830-81-3  
RGT X 7803-57-8 N2H4-H2O  
PRO W 944830-88-0  
CON 1 hour, heated

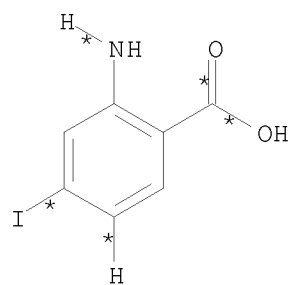
RX(12) RCT E 944830-81-3, W 944830-88-0  
RGT O 127-09-3 AcONa  
PRO AB 944830-90-4  
SOL 64-19-7 AcOH  
CON 18 hours, reflux

RX(114) OF 118 COMPOSED OF REACTION SEQUENCE RX(2), RX(13)  
AND REACTION SEQUENCE RX(1), RX(2), RX(11), RX(13)

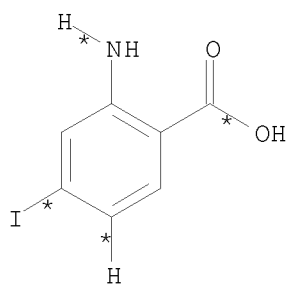
... C ==> E...  
...2 A + 2 B + Y + E ==> AC



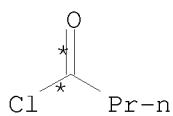
START NEXT REACTION SEQUENCE



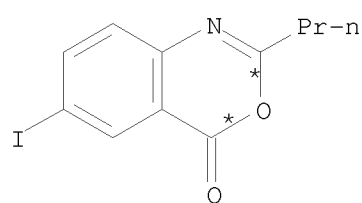
A



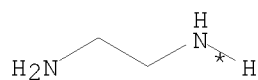
A



2 B

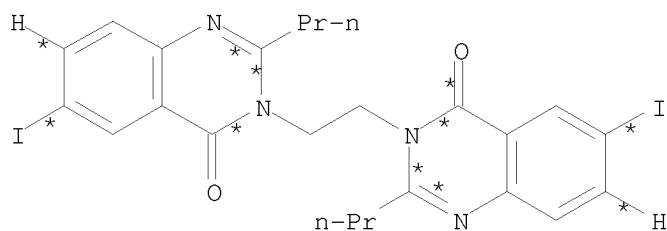


E



Y

4  
STEPS  
→



AC  
YIELD 56%

RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac2O
	CON	4 hours, reflux
RX(1)	RCT	A 20776-54-9, B 141-75-3
	PRO	C 73721-77-4
	SOL	110-86-1 Pyridine
	CON	2 hours, room temperature
RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac2O
	CON	4 hours, reflux
RX(11)	RCT	E 944830-81-3, Y 107-15-3
	PRO	Z 944830-89-1

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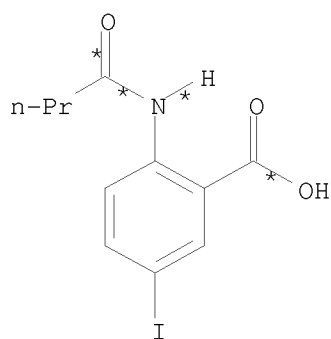
SOL 64-17-5 EtOH  
CON 2 hours, reflux

RX(13) RCT E 944830-81-3, Z 944830-89-1  
RGT O 127-09-3 AcONa  
PRO AC 944830-91-5  
SOL 64-19-7 AcOH  
CON 18 hours, reflux

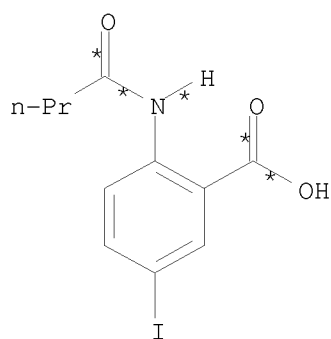
RX(115) OF 118 COMPOSED OF REACTION SEQUENCE RX(2), RX(10), RX(12)  
AND REACTION SEQUENCE RX(1), RX(2), RX(12)

...2 C ==> W...

...A + B + W ==> AB

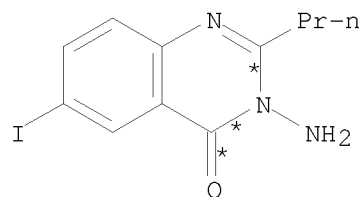


C



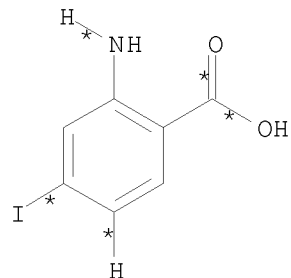
C

3  
STEPS  
→

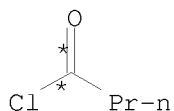


W

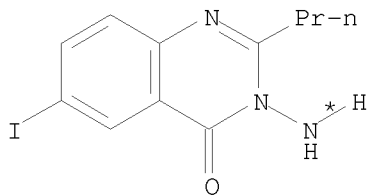
START NEXT REACTION SEQUENCE



A

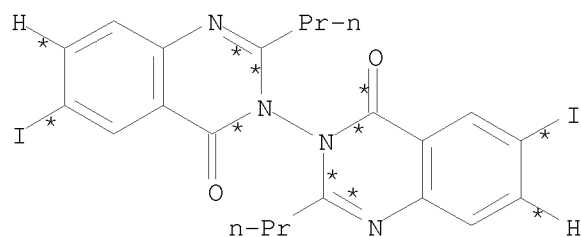


B



W

3  
STEPS  
→



AB  
YIELD 63%

RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(10) RCT E 944830-81-3  
RGT X 7803-57-8 N2H4-H2O  
PRO W 944830-88-0  
CON 1 hour, heated

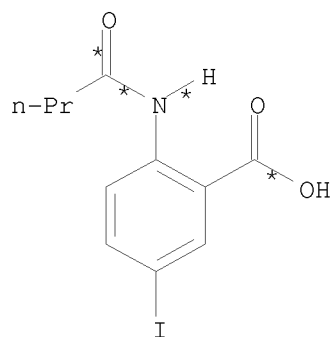
RX(1) RCT A 20776-54-9, B 141-75-3  
PRO C 73721-77-4  
SOL 110-86-1 Pyridine  
CON 2 hours, room temperature

RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

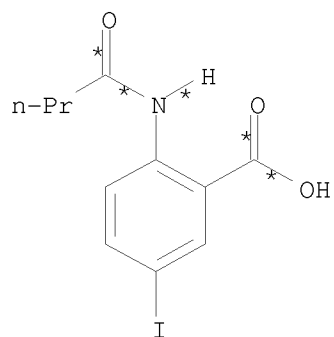
RX(12) RCT E 944830-81-3, W 944830-88-0  
RGT O 127-09-3 AcONa  
PRO AB 944830-90-4  
SOL 64-19-7 AcOH  
CON 18 hours, reflux

RX(116) OF 118 COMPOSED OF REACTION SEQUENCE RX(2), RX(11), RX(13)  
AND REACTION SEQUENCE RX(1), RX(2), RX(13)

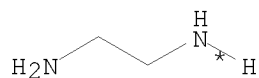
...2 C + Y ==> Z...  
...A + B + Z ==> AC



C

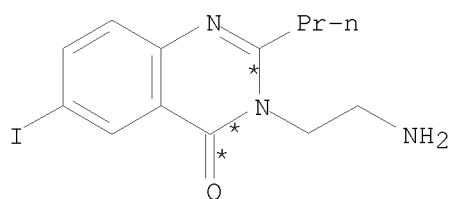


C



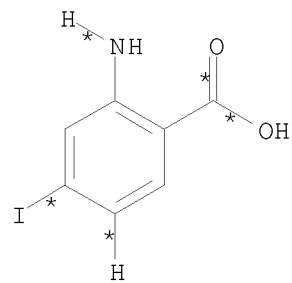
Y

3  
STEPS  
→

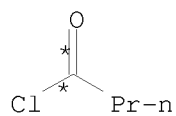


Z

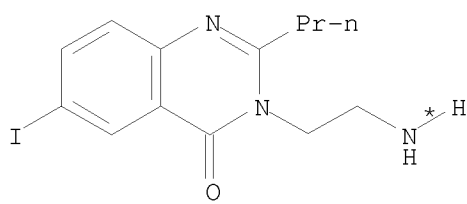
START NEXT REACTION SEQUENCE



A



B

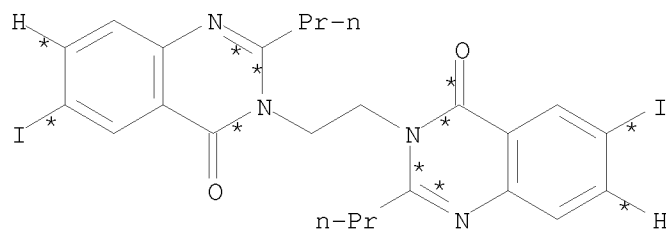


Z

3  
STEPS  
→



10/ 562,112



AC  
YIELD 56%

RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(11) RCT E 944830-81-3, Y 107-15-3  
PRO Z 944830-89-1  
SOL 64-17-5 EtOH  
CON 2 hours, reflux

RX(1) RCT A 20776-54-9, B 141-75-3  
PRO C 73721-77-4  
SOL 110-86-1 Pyridine  
CON 2 hours, room temperature

RX(2) RCT C 73721-77-4  
PRO E 944830-81-3  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(13) RCT E 944830-81-3, Z 944830-89-1  
RGT O 127-09-3 AcONa  
PRO AC 944830-91-5  
SOL 64-19-7 AcOH  
CON 18 hours, reflux

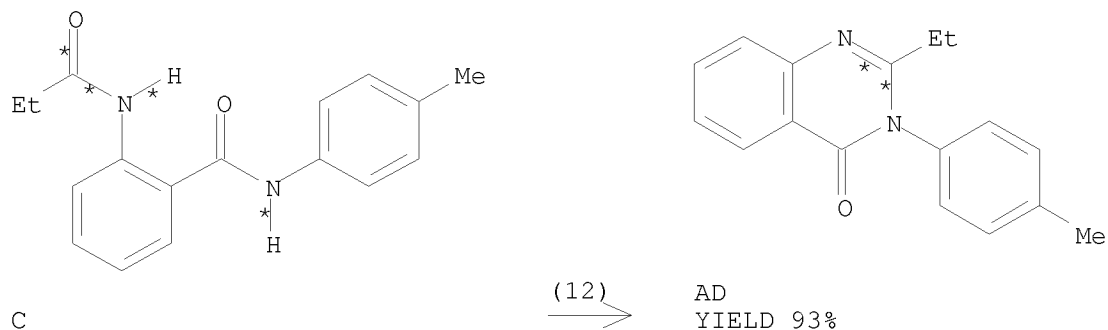
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 20 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 147:52862 CASREACT  
TITLE: Hexamethyldisilazane-iodine induced intramolecular  
dehydrative cyclization of diamides: A general access  
to natural and unnatural quinazolinones  
AUTHOR(S): Kshirsagar, Umesh A.; Mhaske, Santosh B.; Argade,  
Narshinha P.  
CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National  
Chemical Laboratory, Pune, 411 008, India  
SOURCE: Tetrahedron Letters (2007), 48(18), 3243-3246  
CODEN: TELEAY; ISSN: 0040-4039  
PUBLISHER: Elsevier Ltd.  
DOCUMENT TYPE: Journal

LANGUAGE: English

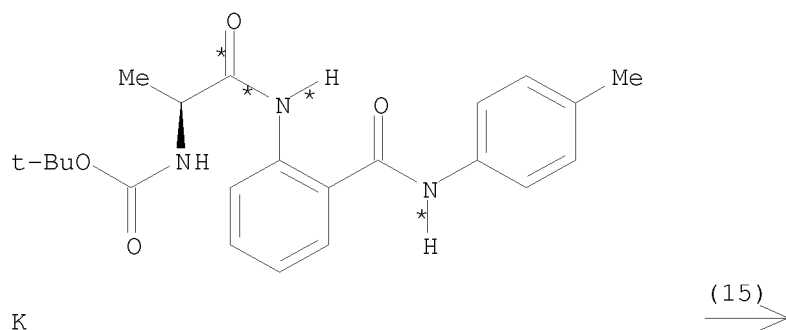
AB A simple and efficient general approach to various quinazolinone scaffolds, including peptidomimetic examples, has been demonstrated by employing hexamethyldisilazane-iodine-induced intramol. dehydrative cyclization of diamides. The N-protecting groups, such as Boc, Fmoc and Cbz, are tolerated and no racemization of optically active substrates was observed. The present protocol has also been used as a key step for the efficient four-step syntheses of the naturally occurring quinazolinones, such as sclerotigenin, (-)-circumdatin-F and (-)-fumiquinazoline-F.

RX(12) OF 45 ...C ==&gt; AD

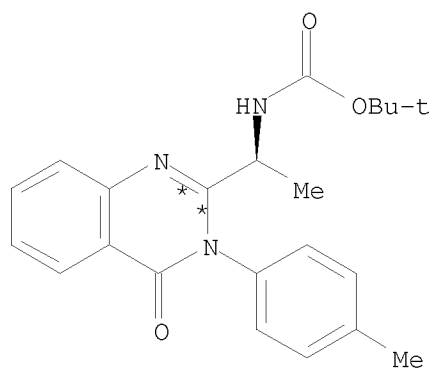


RX(12) RCT C 25628-87-9  
 RGT AE 999-97-3 (Me<sub>3</sub>Si)<sub>2</sub>NH, AF 7553-56-2 I2  
 PRO AD 50498-61-8  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON 30 minutes, room temperature

RX(15) OF 45 ...K ==&gt; AI



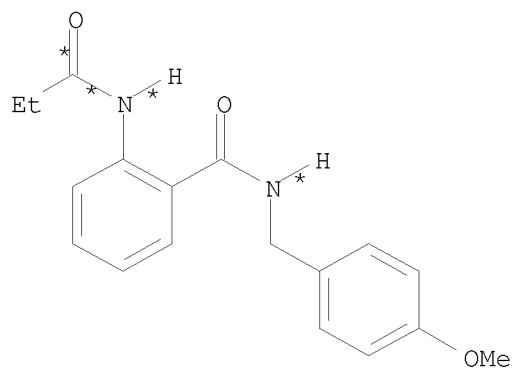
10/ 562,112



AI  
YIELD 70%

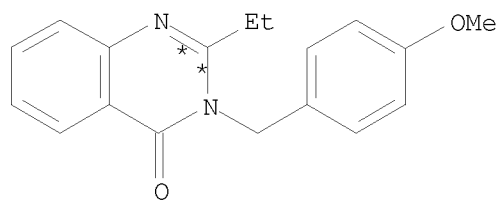
RX(15)      RCT    K 939966-28-6  
              RGT    AE 999-97-3 (Me<sub>3</sub>Si)<sub>2</sub>NH, AF 7553-56-2 I2  
              PRO    AI 939966-46-8  
              SOL    75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
              CON    4 hours, room temperature

RX(16) OF 45      ...O ==> AJ



O

(16)

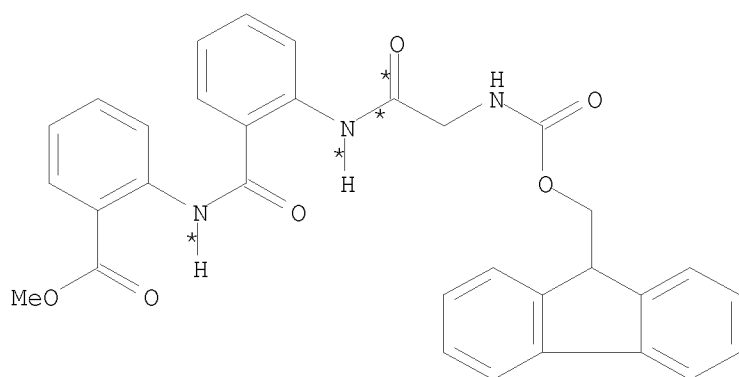


AJ  
YIELD 97%

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RX(16)     RCT   O 939966-30-0  
          RGT   AE 999-97-3 (Me3Si)2NH, AF 7553-56-2 I2  
          PRO   AJ 939966-48-0  
          SOL   75-09-2 CH2Cl2  
          CON   3 hours, room temperature

RX(19) OF 45     ...U ==> AM...



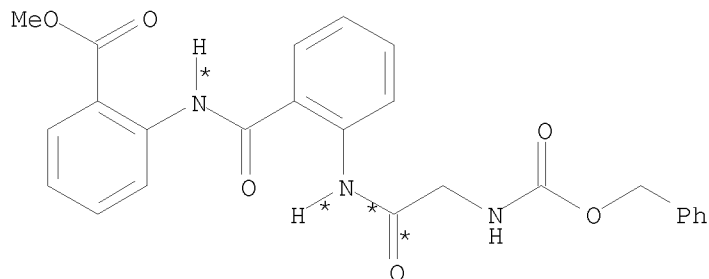
U

(19) →

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(19)     RCT   U 939966-36-6  
          RGT   AE 999-97-3 (Me3Si)2NH, AF 7553-56-2 I2  
          PRO   AM 939966-54-8  
          SOL   75-09-2 CH2Cl2  
          CON   4 hours, room temperature

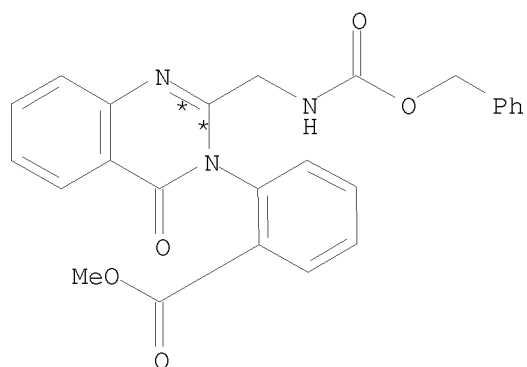
RX(20) OF 45     ...Y ==> AN...



Y

(20) →

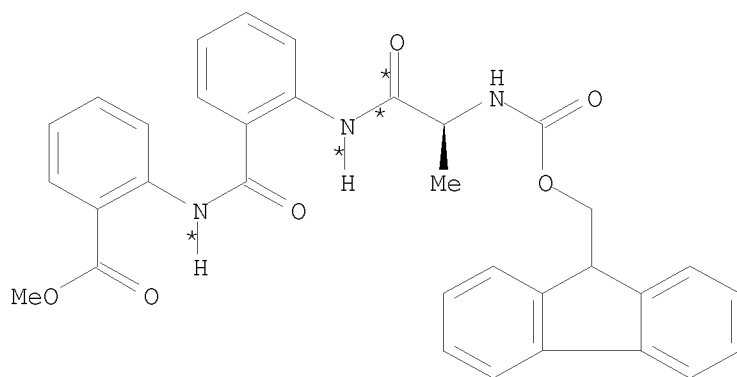
10/ 562,112



AN  
YIELD 65%

RX(20)      RCT    Y 939966-38-8  
             RGT    AE 999-97-3 (Me<sub>3</sub>Si)<sub>2</sub>NH, AF 7553-56-2 I2  
             PRO    AN 939966-56-0  
             SOL    75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
             CON    4 hours, room temperature

RX(21) OF 45      ...AA ==> AO...



AA

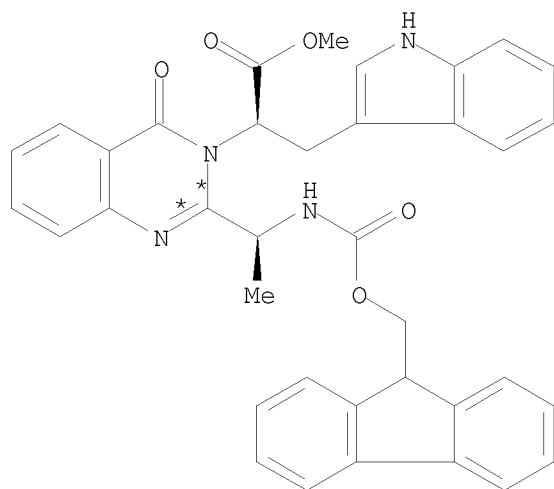
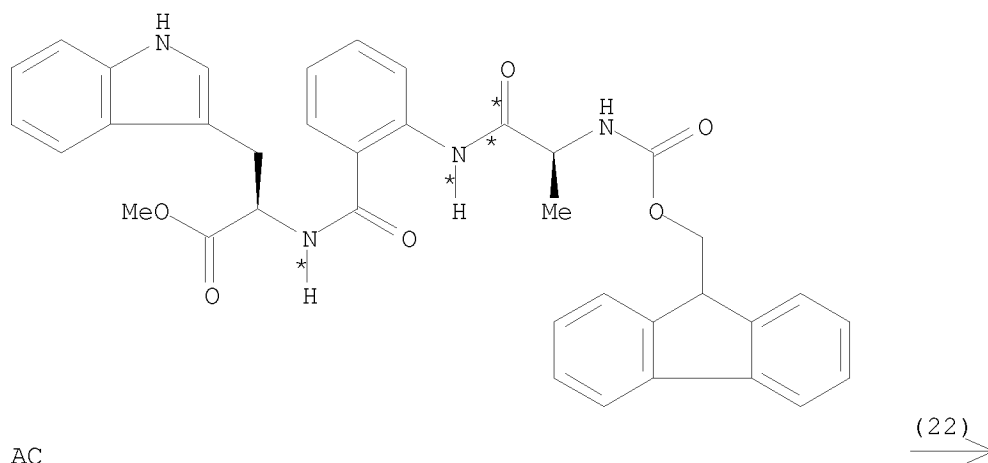
(21)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(21)      RCT    AA 939966-40-2  
             RGT    AE 999-97-3 (Me<sub>3</sub>Si)<sub>2</sub>NH, AF 7553-56-2 I2  
             PRO    AO 939966-58-2  
             SOL    71-43-2 Benzene  
             CON    4 hours, reflux

RX(22) OF 45      ...AC ==> AQ...

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AQ  
YIELD 65%

RX(22) RCT AC 262590-35-2  
RGT AE 999-97-3 (Me<sub>3</sub>Si)<sub>2</sub>NH, AF 7553-56-2 I2  
PRO AQ 939966-60-6  
SOL 71-43-2 Benzene  
CON 3 hours, reflux

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 21 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 146:500996 CASREACT  
TITLE: A Novel Highly Stereoselective Synthesis of  
2,3-Disubstituted 3H-Quinazoline-4-one Derivatives  
AUTHOR(S): Zhichkin, Paul; Kesicki, Edward; Treiberg, Jennifer;

CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE:

LANGUAGE:

GI

Bourdon, Lisa; Ronsheim, Matthew; Ooi, Hua Chee;  
White, Stephen; Judkins, Angela; Fairfax, David  
Albany Molecular Research, Inc., Albany, NY, 12212,  
USA

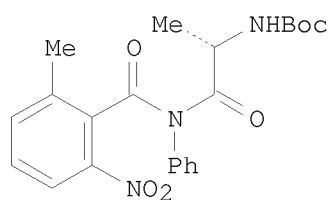
Organic Letters (2007), 9(7), 1415-1418

CODEN: ORLEF7; ISSN: 1523-7060

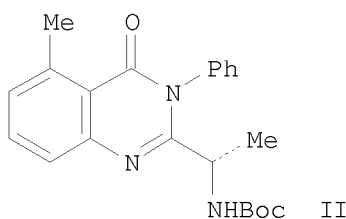
American Chemical Society

Journal

English



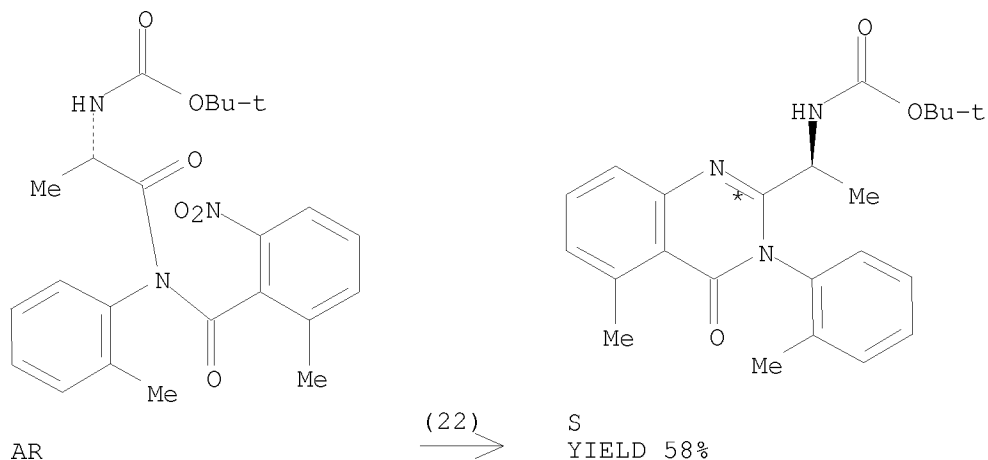
I



II

AB An efficient three-step synthesis of chiral 3H-quinazolin-4-one derivs. from com. materials is disclosed. The Mumm reaction of nitrobenzimidoyl chlorides with chiral L- $\alpha$ -amino acids, which were prepared by chlorination of nitrobenzamides, affords the corresponding (nitrobenzamido)oxoethylcarbamate derivs, e.g., I. Reductive cyclocondensation of the (nitrobenzamido)oxoethylcarbamate derivs affords enantiomerically pure (ee >93%) quinazolin-4-ones, e.g., II, in good overall yield. A comparison with existing approaches indicates that this method is superior for hindered substrates.

RX(22) OF 58 ...AR ==&gt; S

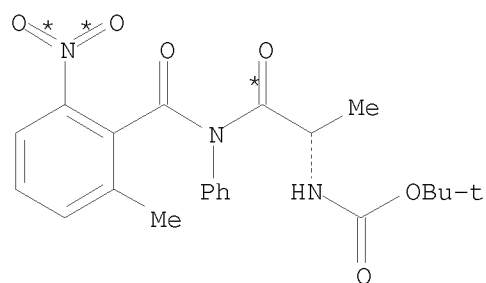


RX(22) RCT AR 936025-18-2  
RGT U 64-19-7 AcOH, BC 7440-66-6 Zn  
PRO S 936024-96-3  
SOL 64-19-7 AcOH  
CON SUBSTAGE(1) 20 deg C

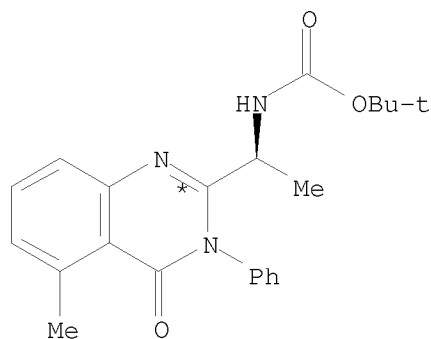
10/ 562,112

SUBSTAGE(2) 3.5 hours, room temperature  
NTE alternative preparation shown, optimized on reducing agents,  
>99% ee, optimization study

RX(23) OF 58 ...AS ==> BD



AS



BD

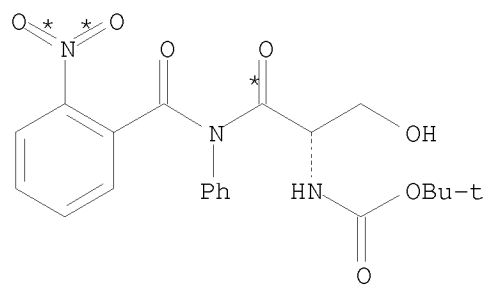
YIELD 60%

RX(23) RCT AS 936025-19-3  
RGT U 64-19-7 AcOH, BC 7440-66-6 Zn  
PRO BD 936025-30-8  
SOL 64-19-7 AcOH  
CON SUBSTAGE(1) 1 hour, room temperature  
SUBSTAGE(2) 3 hours, room temperature  
SUBSTAGE(3) room temperature  
NTE 98% ee, incremental addition of Zn

RX(26) OF 58 ...AZ ==> BG

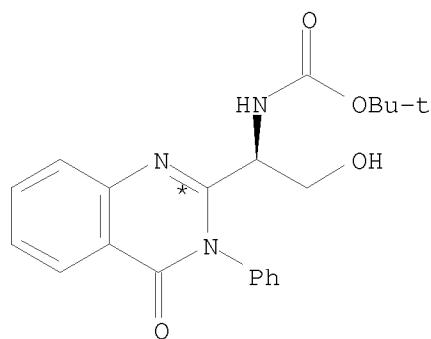


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AZ

(26)

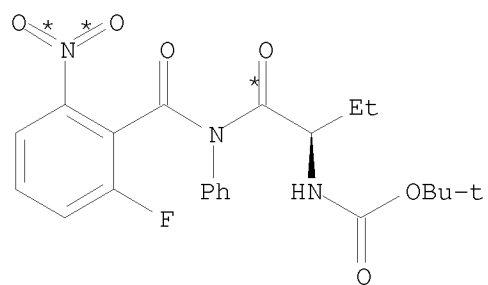


BG

YIELD 57%

RX(26)      RCT    AZ 936025-27-3  
              RGT    U 64-19-7 AcOH, BC 7440-66-6 Zn  
              PRO    BG 936025-35-3  
              SOL    64-19-7 AcOH  
              CON    6 hours, room temperature  
              NTE    94% ee

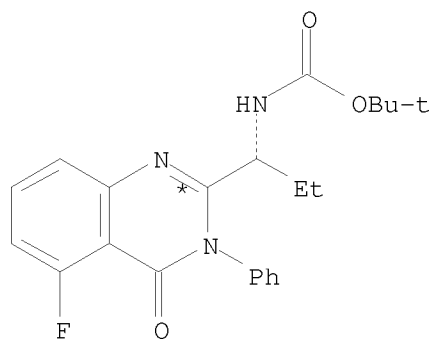
RX(27) OF 58      ...BB ==> BH



BB

(27)

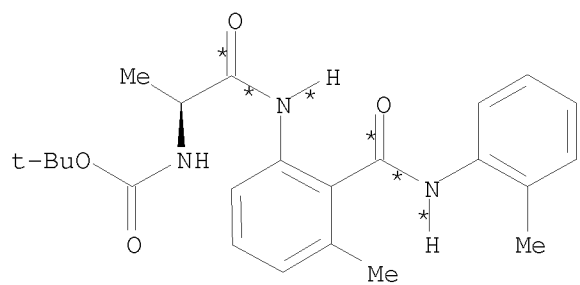
10/ 562,112



BH  
YIELD 67%

RX(27) RCT BB 936025-29-5  
RGT U 64-19-7 AcOH, BC 7440-66-6 Zn  
PRO BH 936025-37-5  
SOL 64-19-7 AcOH  
CON SUBSTAGE(1) 15 minutes, >room temperature  
SUBSTAGE(2) 17.5 hours, room temperature  
NTE >98% ee, incremental addition of Zn

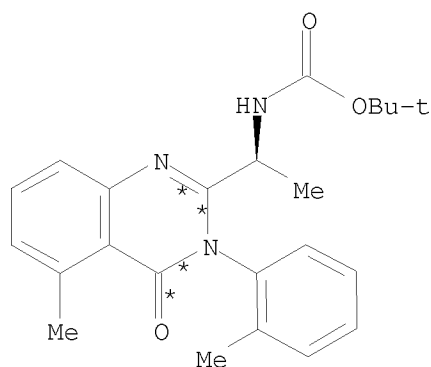
RX(33) OF 58 COMPOSED OF RX(3), RX(4)  
RX(33) J ==> S



J

2  
STEPS  
→

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S  
YIELD 94%

RX(3)

STAGE(1)

RGT O 7726-95-6 Br<sub>2</sub>, P 603-35-0 PPh<sub>3</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 30 minutes, room temperature

STAGE(2)

RCT J 936024-93-0  
RGT Q 121-44-8 Et<sub>3</sub>N  
CON SUBSTAGE(1) reflux  
SUBSTAGE(2) 1.5 hours, reflux

PRO N 936024-94-1  
NTE stage 2 exothermic

RX(4) RCT N 936024-94-1

STAGE(1)

RGT T 123-75-1 Pyrrolidine  
SOL 123-75-1 Pyrrolidine  
CON overnight, room temperature

STAGE(2)

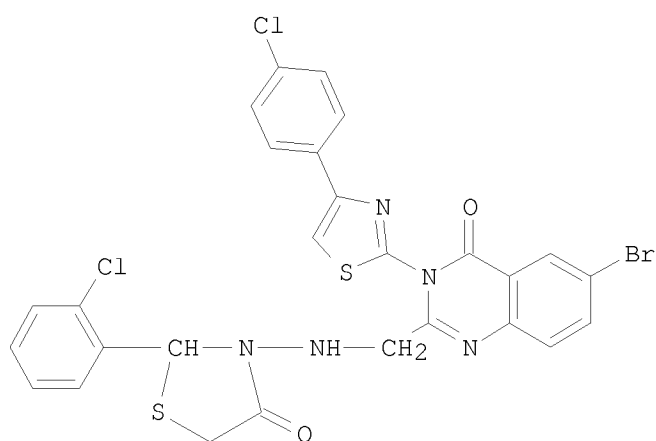
RGT U 64-19-7 AcOH  
SOL 75-05-8 MeCN  
CON 30 minutes, reflux

PRO S 936024-96-3  
NTE alternative preparation shown, 96% ee, 14% overall yield for 3 steps

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 22 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 146:474765 CASREACT

TITLE: Synthesis of 3-[4'-(p-chlorophenyl)-thiazol-2'-yl]-2-  
 [(substituted azetidinone/thiazolidinone)-aminomethyl]-  
 6-bromoquinazolin-4-ones as anti-inflammatory agent  
 AUTHOR(S): Kumar, Ashok; Rajput, Chatrasal Singh; Bhati, Sudhir  
 Kumar  
 CORPORATE SOURCE: Department of Pharmacology, L L R M Medical College,  
 Meerut (UP), 250004, India  
 SOURCE: Bioorganic & Medicinal Chemistry (2007), 15(8),  
 3089-3096  
 CODEN: BMECEP; ISSN: 0968-0896  
 PUBLISHER: Elsevier Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

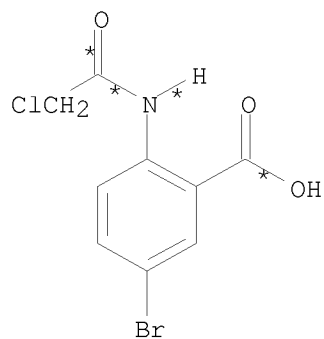


I

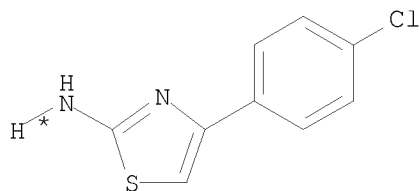
AB Title compds. were prepared and screened for anti-inflammatory and analgesic activities at the dose of 50 mg/kg po. Compound 21 (I) showed maximum anti-inflammatory (38.35%) and analgesic (37.36%) activities. Compound 21 was also tested for ulcerogenic activity and the UD50 value was found to be 195.6 mg/kg po.

RX(2) OF 118 ...C + F ==> G...

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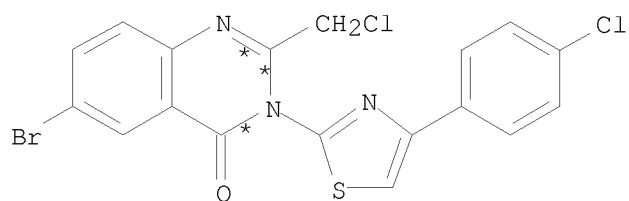


C



F

(2)  $\longrightarrow$

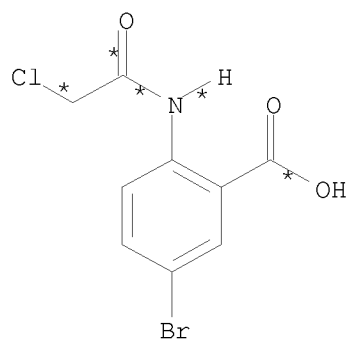


G

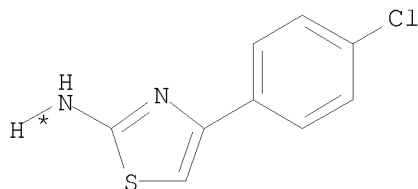
YIELD 55%

RX(2) RCT C 155104-20-4, F 2103-99-3  
 RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO G 935702-18-4  
 SOL 71-43-2 Benzene  
 CON 2 hours, reflux

RX(29) OF 118 COMPOSED OF RX(2), RX(3)  
 RX(29) C + F  $\implies$  I



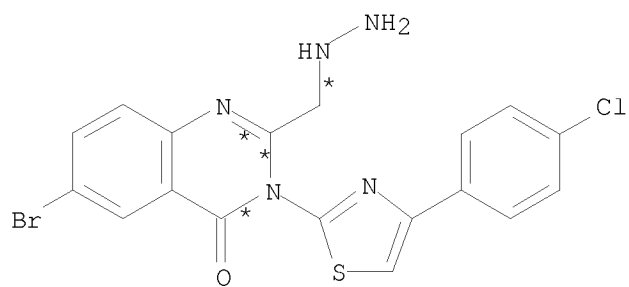
C



F

2  
 STEPS  
 $\longrightarrow$

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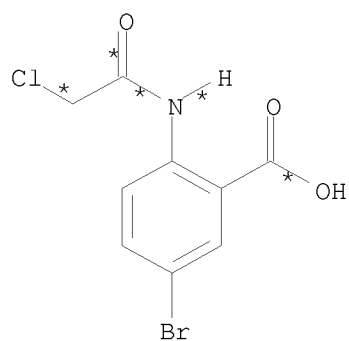


I  
YIELD 62%

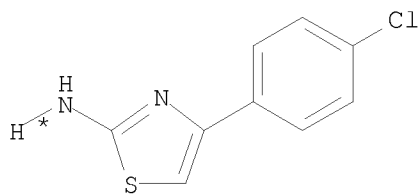
RX(2)        RCT    C 155104-20-4, F 2103-99-3  
              RGT    H 584-08-7 K2CO3  
              PRO    G 935702-18-4  
              SOL    71-43-2 Benzene  
              CON    2 hours, reflux

RX(3)        RCT    G 935702-18-4  
              RGT    J 7803-57-8 N2H4-H2O  
              PRO    I 935702-19-5  
              SOL    64-17-5 EtOH  
              CON    10 hours, reflux

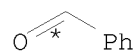
RX(55) OF 118 COMPOSED OF RX(2), RX(3), RX(4)  
RX(55)       C   +   F   +   L   ==>   M



C



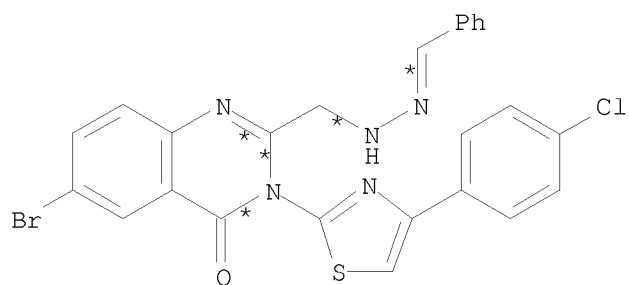
F



L

3  
STEPS  
→

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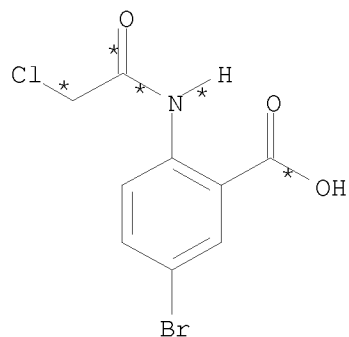
M  
YIELD 65%

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

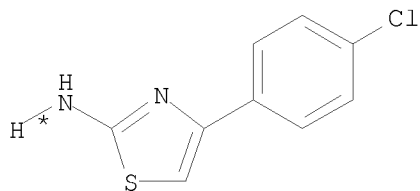
RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N<sub>2</sub>H<sub>4</sub>·H<sub>2</sub>O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

RX(4) RCT I 935702-19-5, L 100-52-7  
PRO M 935702-20-8  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 8 hours, reflux

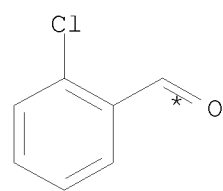
RX(56) OF 118 COMPOSED OF RX(2), RX(3), RX(5)  
RX(56) C + F + O ==> P



C



F



O

3  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

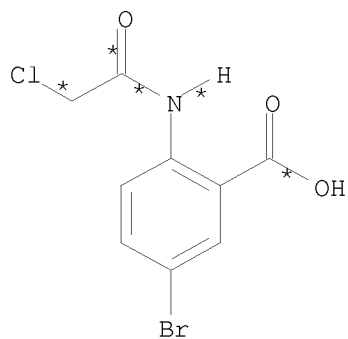
RX(2) RCT C 155104-20-4, F 2103-99-3  
 RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO G 935702-18-4  
 SOL 71-43-2 Benzene  
 CON 2 hours, reflux

RX(3) RCT G 935702-18-4  
 RGT J 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
 PRO I 935702-19-5  
 SOL 64-17-5 EtOH  
 CON 10 hours, reflux

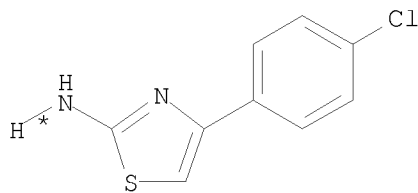
RX(5) RCT I 935702-19-5, O 89-98-5  
 PRO P 935702-21-9  
 CAT 64-19-7 AcOH  
 SOL 64-17-5 EtOH  
 CON reflux

RX(57) OF 118 COMPOSED OF RX(2), RX(3), RX(6)

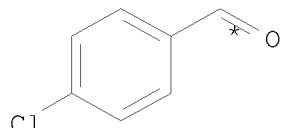
RX(57) C + F + Q ==> R



C



F

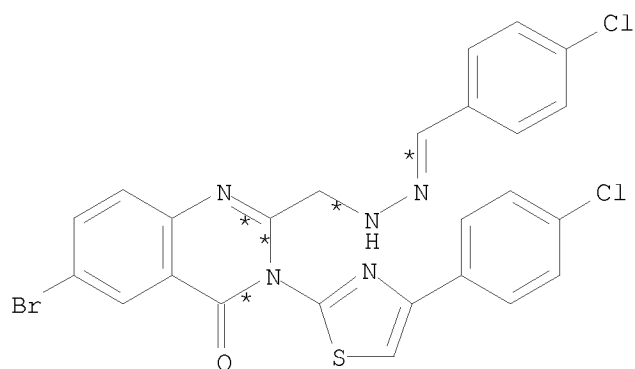


Q

3  
 STEPS  
 →



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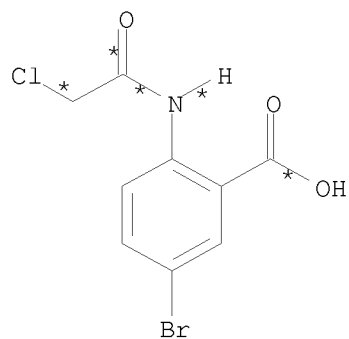
R  
YIELD 58%

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

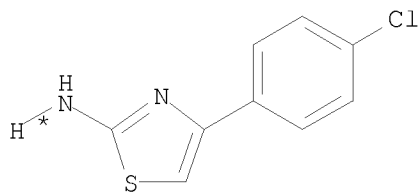
RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

RX(6) RCT I 935702-19-5, Q 104-88-1  
PRO R 935702-22-0  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON reflux

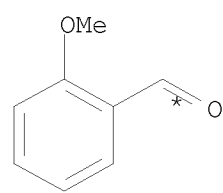
RX(58) OF 118 COMPOSED OF RX(2), RX(3), RX(7)  
RX(58) C + F + S ==> T



C



F



S

10/ 562,112

3

STEPS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

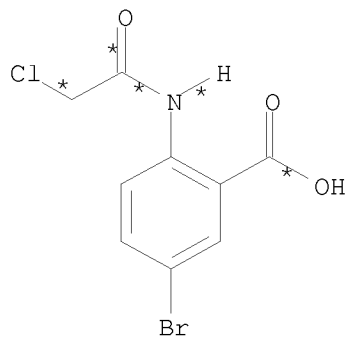
RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N<sub>2</sub>H<sub>4</sub>·H<sub>2</sub>O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

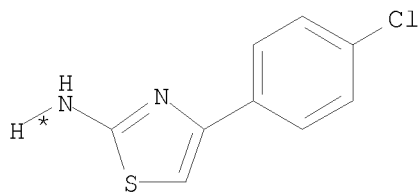
RX(7) RCT I 935702-19-5, S 135-02-4  
PRO T 935702-23-1  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON reflux

RX(59) OF 118 COMPOSED OF RX(2), RX(3), RX(8)

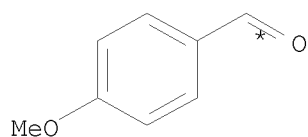
RX(59) C + F + U ==> V



C



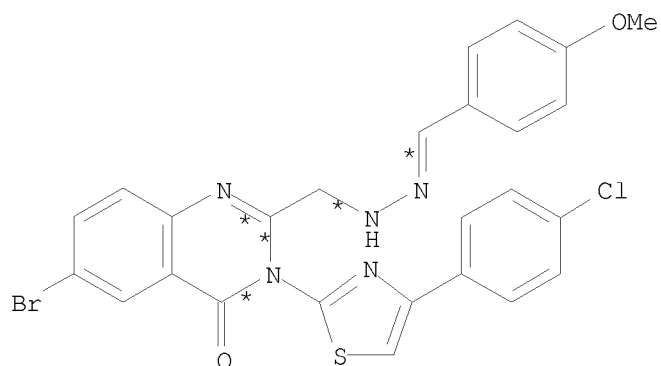
F



U

3  
STEPS  
→

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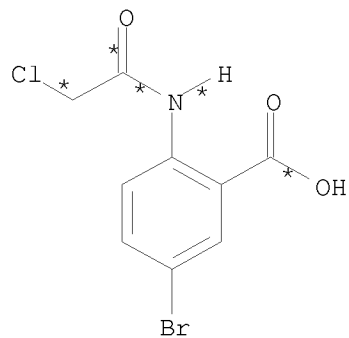
V  
YIELD 60%

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

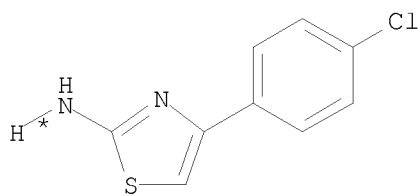
RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

RX(8) RCT I 935702-19-5, U 123-11-5  
PRO V 935702-24-2  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON reflux

RX(60) OF 118 COMPOSED OF RX(2), RX(3), RX(9)  
RX(60) C + F + W ==> X

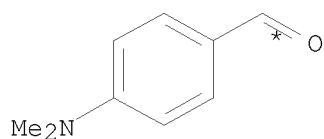


C



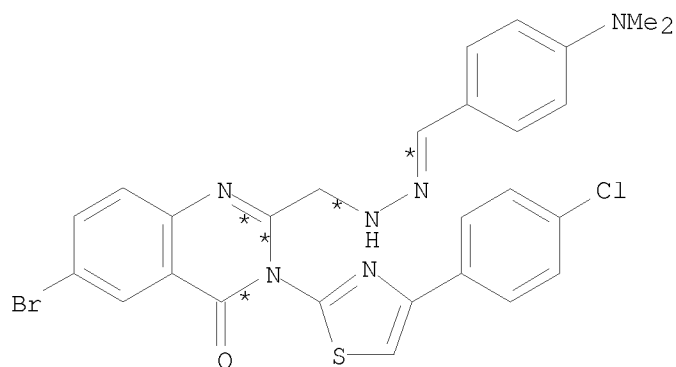
F

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W

3  
STEPS  
→



X

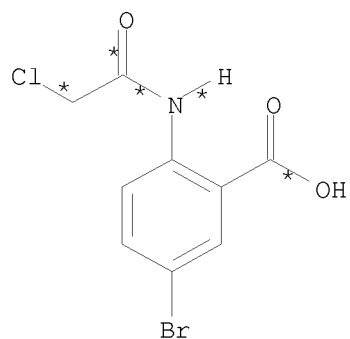
YIELD 65%

RX(2)      RCT    C 155104-20-4, F 2103-99-3  
            RGT    H 584-08-7 K2CO3  
            PRO    G 935702-18-4  
            SOL    71-43-2 Benzene  
            CON    2 hours, reflux

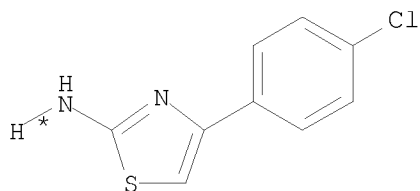
RX(3)      RCT    G 935702-18-4  
            RGT    J 7803-57-8 N2H4-H2O  
            PRO    I 935702-19-5  
            SOL    64-17-5 EtOH  
            CON    10 hours, reflux

RX(9)      RCT    I 935702-19-5, W 100-10-7  
            PRO    X 935702-25-3  
            CAT    64-19-7 AcOH  
            SOL    64-17-5 EtOH  
            CON    reflux

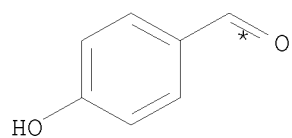
RX(61) OF 118 COMPOSED OF RX(2), RX(3), RX(10)  
RX(61)      C    +    F    +    Y    ==>    Z



C

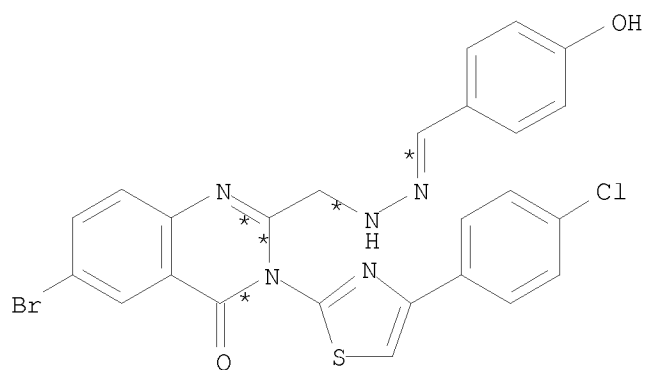


F



Y

3  
STEPS  
→



Z

YIELD 62%

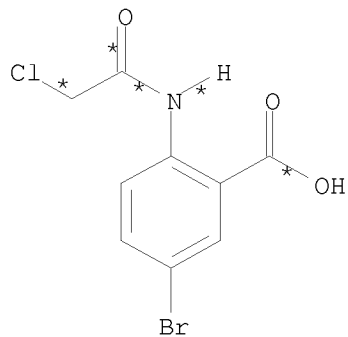
RX(2) RCT C 155104-20-4, F 2103-99-3  
 RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO G 935702-18-4  
 SOL 71-43-2 Benzene  
 CON 2 hours, reflux

RX(3) RCT G 935702-18-4  
 RGT J 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
 PRO I 935702-19-5  
 SOL 64-17-5 EtOH  
 CON 10 hours, reflux

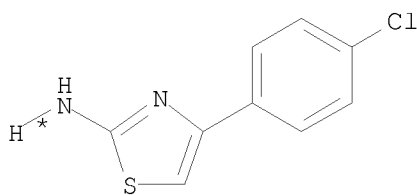
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RX(10)      RCT    I 935702-19-5, Y 123-08-0  
              PRO    Z 935702-26-4  
              CAT    64-19-7 AcOH  
              SOL    64-17-5 EtOH  
              CON    reflux

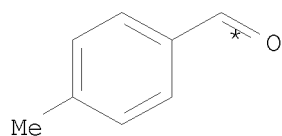
RX(62) OF 118 COMPOSED OF RX(2), RX(3), RX(11)  
RX(62)      C   +   F   +   AA   ==>   AB



C

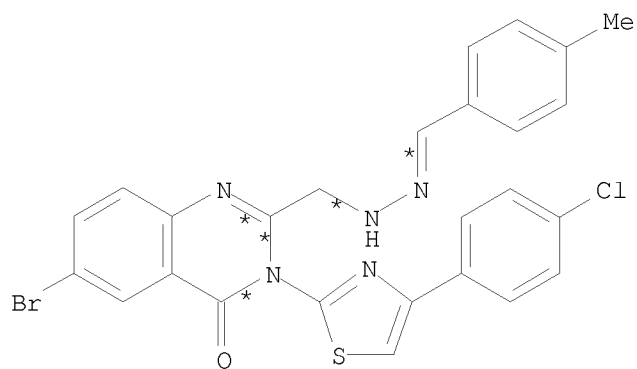


F



AA

3  
STEPS  
→



AB

YIELD 59%

RX(2)      RCT    C 155104-20-4, F 2103-99-3

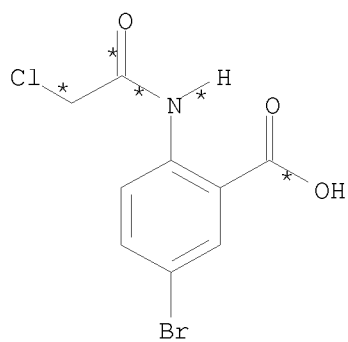
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RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

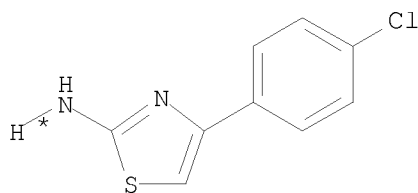
RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N<sub>2</sub>H<sub>4</sub>·H<sub>2</sub>O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

RX(11) RCT I 935702-19-5, AA 104-87-0  
PRO AB 935702-27-5  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON reflux

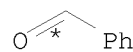
RX(87) OF 118 COMPOSED OF RX(2), RX(3), RX(4), RX(12)  
RX(87) C + F + L + B ==> AC



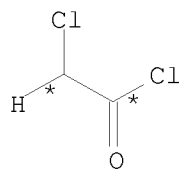
C



F

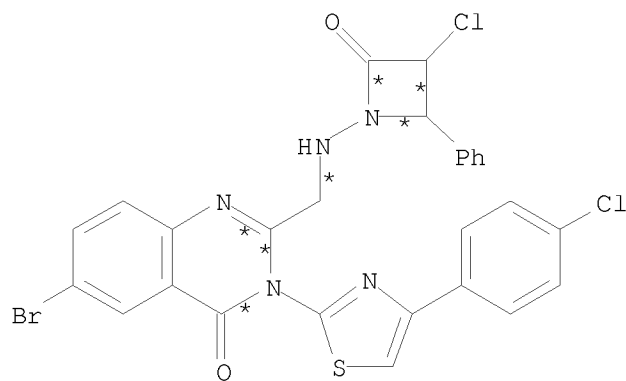


L



B

4  
STEPS  
→



AC  
YIELD 55%

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>

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PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

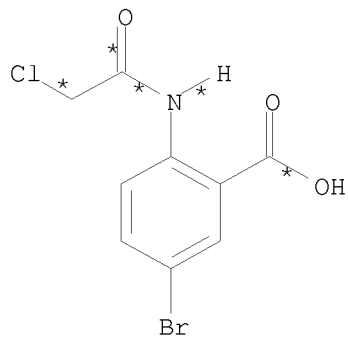
RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N2H4-H2O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

RX(4) RCT I 935702-19-5, L 100-52-7  
PRO M 935702-20-8  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 8 hours, reflux

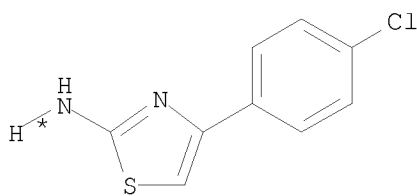
RX(12) RCT M 935702-20-8, B 79-04-9  
RGT AD 121-44-8 Et3N  
PRO AC 935702-28-6  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 40 minutes, room temperature  
SUBSTAGE(3) 7 hours, reflux

RX(88) OF 118 COMPOSED OF RX(2), RX(3), RX(4), RX(20)

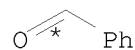
RX(88) C + F + L + AL ==> AM



C



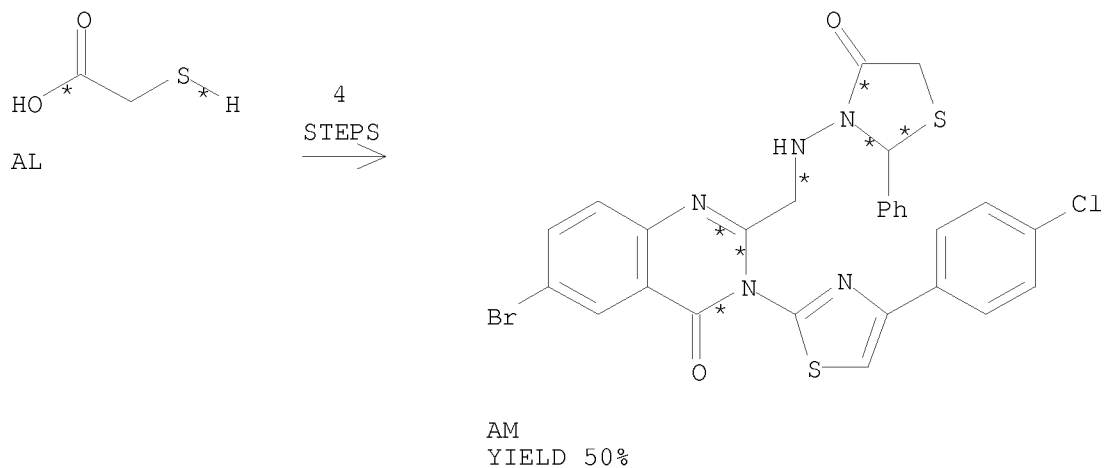
F



L



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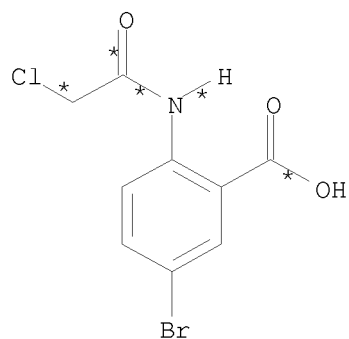
RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K2CO3  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N2H4-H2O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

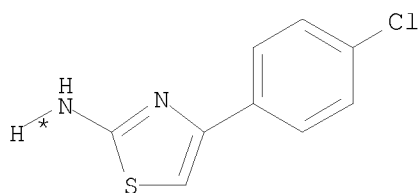
RX(4) RCT I 935702-19-5, L 100-52-7  
PRO M 935702-20-8  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON 8 hours, reflux

RX(20) RCT M 935702-20-8, AL 68-11-1  
PRO AM 935702-36-6  
CAT 7646-85-7 ZnCl2  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 3 days, room temperature  
SUBSTAGE(3) 14 hours, reflux

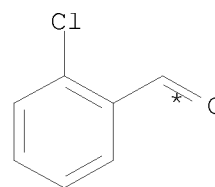
RX(89) OF 118 COMPOSED OF RX(2), RX(3), RX(5), RX(13)  
RX(89) C + F + O + B ==> AE



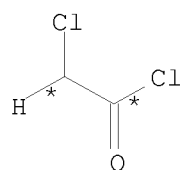
C



F



O



B

4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N<sub>2</sub>H<sub>4</sub>·H<sub>2</sub>O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

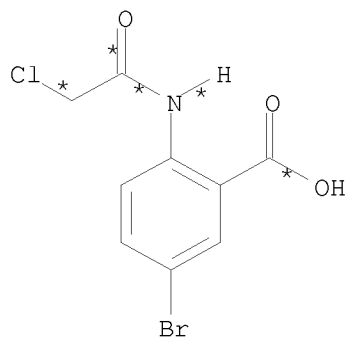
RX(5) RCT I 935702-19-5, O 89-98-5  
PRO P 935702-21-9  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON reflux

RX(13) RCT P 935702-21-9, B 79-04-9  
RGT AD 121-44-8 Et<sub>3</sub>N  
PRO AE 935702-29-7  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) room temperature  
SUBSTAGE(3) reflux

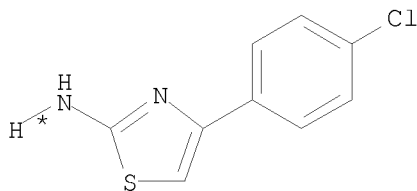
RX(90) OF 118 COMPOSED OF RX(2), RX(3), RX(5), RX(21)

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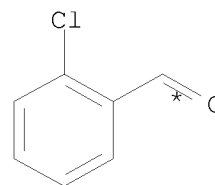
RX(90) C + F + O + AL ==> AO



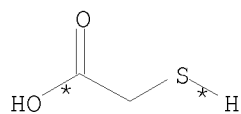
C



F



O



AL

4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K2CO3  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

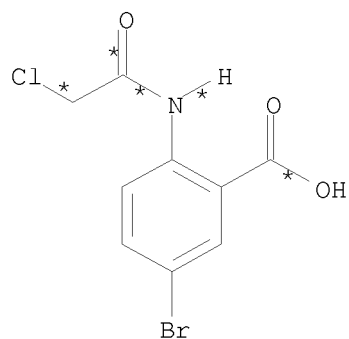
RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N2H4-H2O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

RX(5) RCT I 935702-19-5, O 89-98-5  
PRO P 935702-21-9  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON reflux

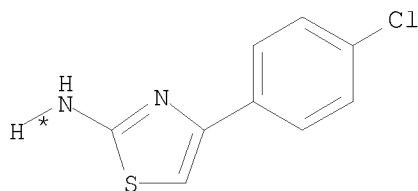
RX(21) RCT P 935702-21-9, AL 68-11-1  
PRO AO 935702-37-7  
CAT 7646-85-7 ZnCl2  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) reflux

RX(91) OF 118 COMPOSED OF RX(2), RX(3), RX(6), RX(14)

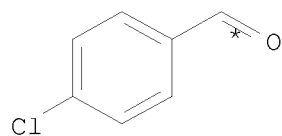
RX(91) C + F + Q + B ==> AF



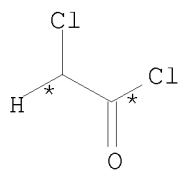
C



F



Q



B

4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

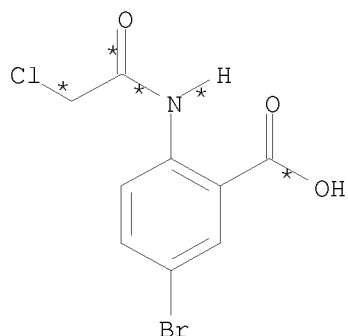
RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

RX(6) RCT I 935702-19-5, Q 104-88-1  
PRO R 935702-22-0  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON reflux

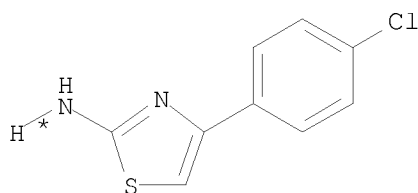
RX(14) RCT R 935702-22-0, B 79-04-9  
RGT AD 121-44-8 Et<sub>3</sub>N  
PRO AF 935702-30-0  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) room temperature  
SUBSTAGE(3) reflux

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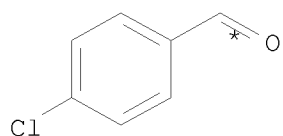
RX(92) OF 118 COMPOSED OF RX(2), RX(3), RX(6), RX(22)  
RX(92) C + F + Q + AL ==> AP



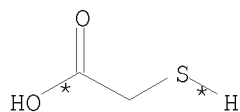
C



F



Q



AL

4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K2CO3  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

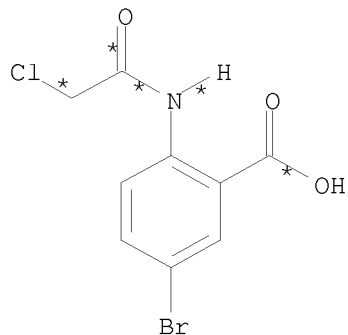
RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N2H4-H2O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

RX(6) RCT I 935702-19-5, Q 104-88-1  
PRO R 935702-22-0  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON reflux

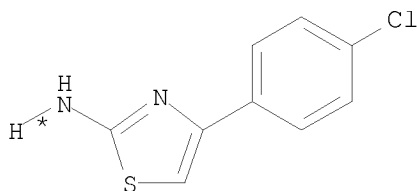
RX(22) RCT R 935702-22-0, AL 68-11-1  
PRO AP 935702-38-8  
CAT 7646-85-7 ZnCl2  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) reflux

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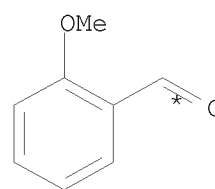
RX(93) OF 118 COMPOSED OF RX(2), RX(3), RX(7), RX(15)  
RX(93) C + F + S + B ==> AG



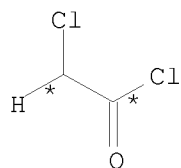
C



F



S



B

4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

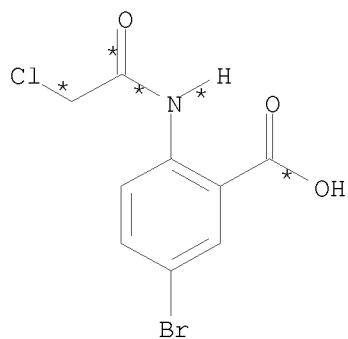
RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

RX(7) RCT I 935702-19-5, S 135-02-4  
PRO T 935702-23-1  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON reflux

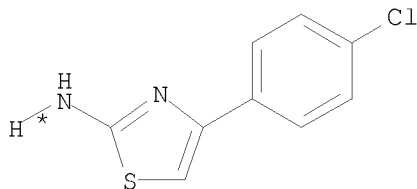
RX(15) RCT T 935702-23-1, B 79-04-9  
RGT AD 121-44-8 Et<sub>3</sub>N  
PRO AG 935702-31-1  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) room temperature  
SUBSTAGE(3) reflux

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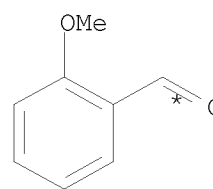
RX(94) OF 118 COMPOSED OF RX(2), RX(3), RX(7), RX(23)  
RX(94) C + F + S + AL ==> AQ



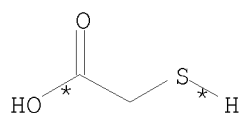
C



F



S



AL

4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K2CO3  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

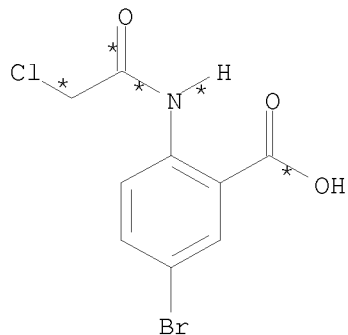
RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N2H4-H2O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

RX(7) RCT I 935702-19-5, S 135-02-4  
PRO T 935702-23-1  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON reflux

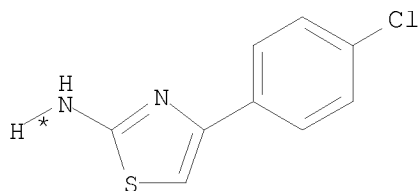
RX(23) RCT T 935702-23-1, AL 68-11-1  
PRO AQ 935702-39-9  
CAT 7646-85-7 ZnCl2  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) reflux

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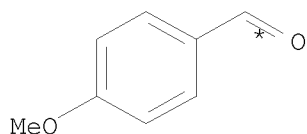
RX(95) OF 118 COMPOSED OF RX(2), RX(3), RX(8), RX(16)  
RX(95) C + F + U + B ==> AH



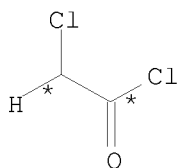
C



F



U



B

4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N<sub>2</sub>H<sub>4</sub>·H<sub>2</sub>O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

RX(8) RCT I 935702-19-5, U 123-11-5  
PRO V 935702-24-2  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON reflux

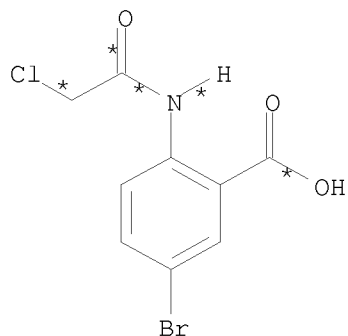
RX(16) RCT V 935702-24-2, B 79-04-9  
RGT AD 121-44-8 Et<sub>3</sub>N  
PRO AH 935702-32-2  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) room temperature



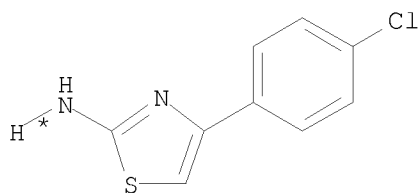
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SUBSTAGE(3) reflux

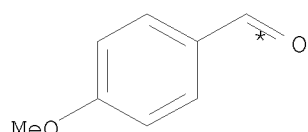
RX(96) OF 118 COMPOSED OF RX(2), RX(3), RX(8), RX(24)  
RX(96) C + F + U + AL ==> AR



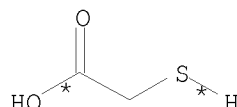
C



F



U



AL

4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K2CO3  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N2H4-H2O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

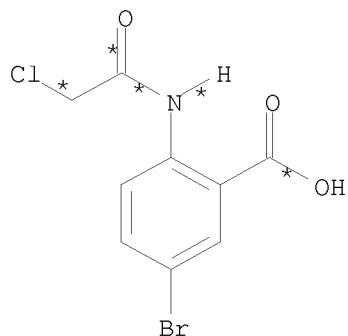
RX(8) RCT I 935702-19-5, U 123-11-5  
PRO V 935702-24-2  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON reflux

RX(24) RCT V 935702-24-2, AL 68-11-1  
PRO AR 935702-40-2  
CAT 7646-85-7 ZnCl2  
SOL 71-43-2 Benzene

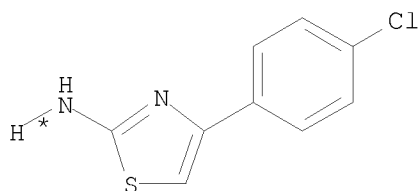
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CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) reflux

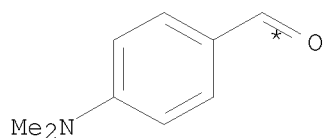
RX(97) OF 118 COMPOSED OF RX(2), RX(3), RX(9), RX(17)  
RX(97) C + F + W + B ==> AI



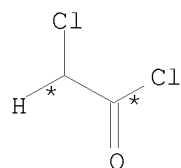
C



F



W



B

4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

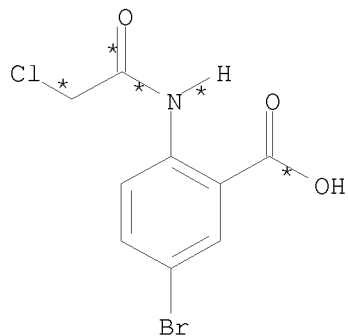
RX(9) RCT I 935702-19-5, W 100-10-7  
PRO X 935702-25-3  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON reflux

RX(17) RCT X 935702-25-3, B 79-04-9  
RGT AD 121-44-8 Et<sub>3</sub>N  
PRO AI 935702-33-3

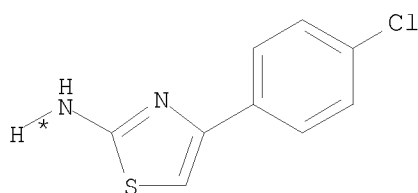
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SOL 71-43-2 Benzene  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) room temperature  
SUBSTAGE(3) reflux

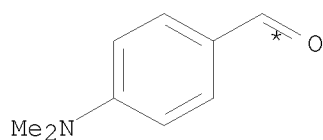
RX(98) OF 118 COMPOSED OF RX(2), RX(3), RX(9), RX(25)  
RX(98) C + F + W + AL ==> AS



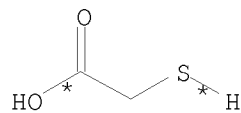
C



F



W



AL

4  
STEPS  
➔

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N<sub>2</sub>H<sub>4</sub>·H<sub>2</sub>O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

RX(9) RCT I 935702-19-5, W 100-10-7  
PRO X 935702-25-3  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON reflux

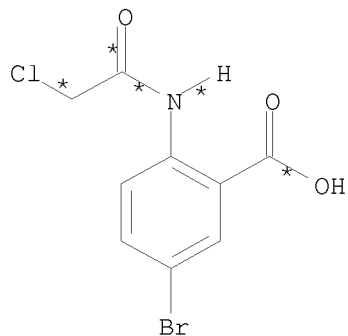
RX(25) RCT X 935702-25-3, AL 68-11-1

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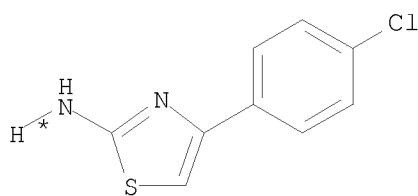
PRO AS 935702-41-3  
CAT 7646-85-7 ZnCl<sub>2</sub>  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) reflux

RX(99) OF 118 COMPOSED OF RX(2), RX(3), RX(10), RX(18)

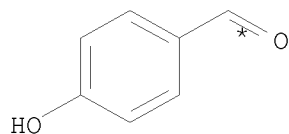
RX(99) C + F + Y + B ==> AJ



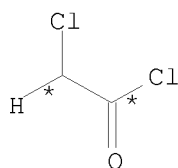
C



F



Y



B

4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

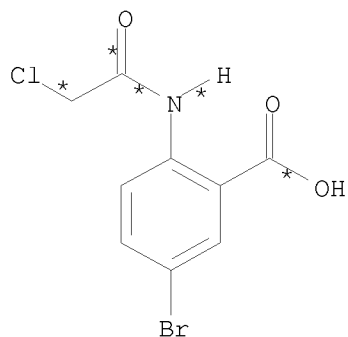
RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

RX(10) RCT I 935702-19-5, Y 123-08-0  
PRO Z 935702-26-4  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON reflux

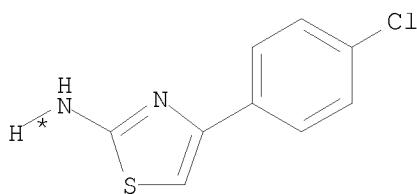
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RX(18) RCT Z 935702-26-4, B 79-04-9  
RGT AD 121-44-8 Et3N  
PRO AJ 935702-34-4  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) room temperature  
SUBSTAGE(3) reflux

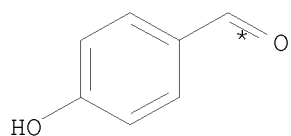
RX(100) OF 118 COMPOSED OF RX(2), RX(3), RX(10), RX(26)  
RX(100) C + F + Y + AL ==> AT



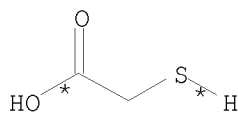
C



F



Y



AL

4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K2CO3  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N2H4-H2O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

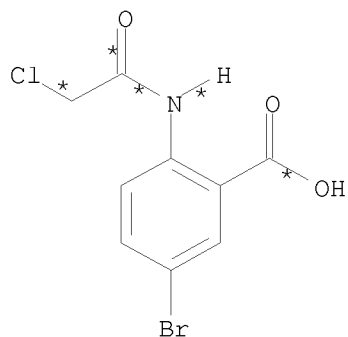
RX(10) RCT I 935702-19-5, Y 123-08-0  
PRO Z 935702-26-4  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH

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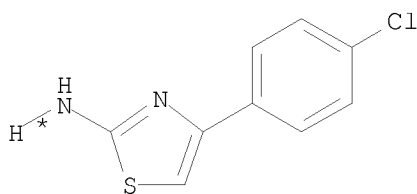
CON reflux

RX(26) RCT Z 935702-26-4, AL 68-11-1  
PRO AT 935702-42-4  
CAT 7646-85-7 ZnCl2  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) reflux

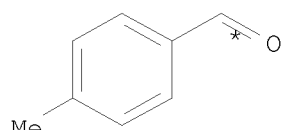
RX(101) OF 118 COMPOSED OF RX(2), RX(3), RX(11), RX(19)  
RX(101) C + F + AA + B ==> AK



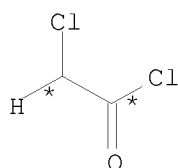
C



F



AA



B

4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K2CO3  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N2H4-H2O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

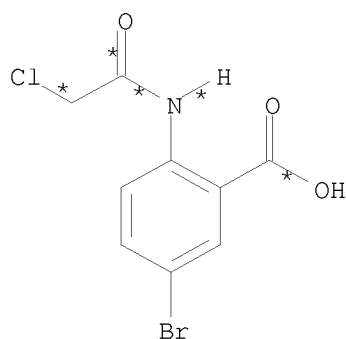
RX(11) RCT I 935702-19-5, AA 104-87-0  
PRO AB 935702-27-5  
CAT 64-19-7 AcOH

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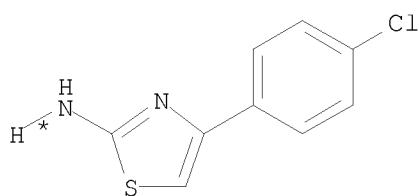
SOL 64-17-5 EtOH  
CON reflux

RX(19) RCT AB 935702-27-5, B 79-04-9  
RGT AD 121-44-8 Et3N  
PRO AK 935702-35-5  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) room temperature  
SUBSTAGE(3) reflux

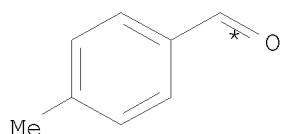
RX(102) OF 118 COMPOSED OF RX(2), RX(3), RX(11), RX(27)  
RX(102) C + F + AA + AL ==> AU



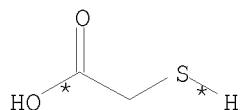
C



F



AA



AL

4  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 155104-20-4, F 2103-99-3  
RGT H 584-08-7 K2CO3  
PRO G 935702-18-4  
SOL 71-43-2 Benzene  
CON 2 hours, reflux

RX(3) RCT G 935702-18-4  
RGT J 7803-57-8 N2H4-H2O  
PRO I 935702-19-5  
SOL 64-17-5 EtOH  
CON 10 hours, reflux

RX(11) RCT I 935702-19-5, AA 104-87-0

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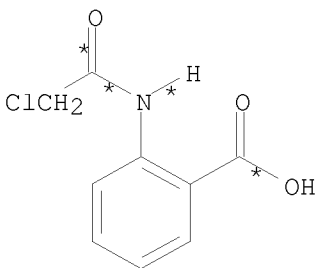
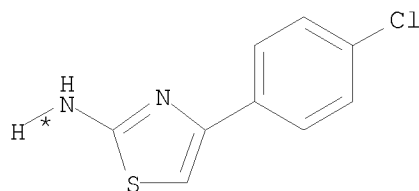
PRO AB 935702-27-5  
CAT 64-19-7 AcOH  
SOL 64-17-5 EtOH  
CON reflux

RX(27) RCT AB 935702-27-5, AL 68-11-1  
PRO AU 935702-43-5  
CAT 7646-85-7 ZnCl2  
SOL 71-43-2 Benzene  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) reflux

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 23 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 146:462201 CASREACT  
TITLE: Synthesis of N-3(4-(4-chlorophenylthiazole-2-yl)-(2-(amino)methyl)-quinazoline-4(3H)-one and their derivatives for antitubercular activity  
AUTHOR(S): Pattan, Shashikant R.; Reddy, V. V. Krishna; Manvi, F. V.; Desai, B. G.; Bhat, A. R.  
CORPORATE SOURCE: Department of Medicinal Chemistry, K L E S's College of Pharmacy, Belgaum, 590 010, Belg.  
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2006), 45B(7), 1778-1781  
CODEN: IJSBDB; ISSN: 0376-4699  
PUBLISHER: National Institute of Science Communication and Information Resources  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB A new series of N-3[4-(4-chlorophenylthiazole-2-yl)-2-aminomethyl]quinazoline-4(3H)-one and their derivs. are synthesized. The structures of the title compds. are confirmed on the basis of IR and <sup>1</sup>H NMR. The compds. are screened for their antitubercular activity, using H37Rv strain on L J medium. All the compds. have showed moderate to promising antitubercular activity.

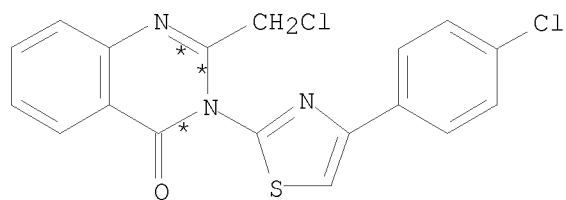
RX(3) OF 56 ...C + H ==> K...



(3) >



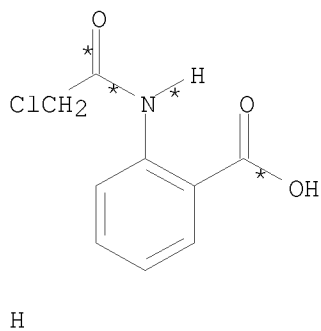
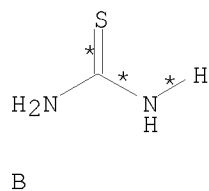
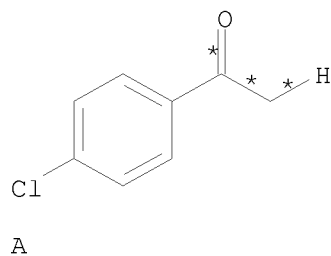
10/ 562,112



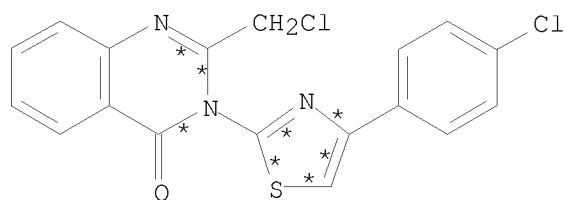
K  
YIELD 58%

RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

RX(14) OF 56 COMPOSED OF RX(1), RX(3)  
RX(14) A + B + H ==> K



2  
STEPS  
→



K  
YIELD 58%

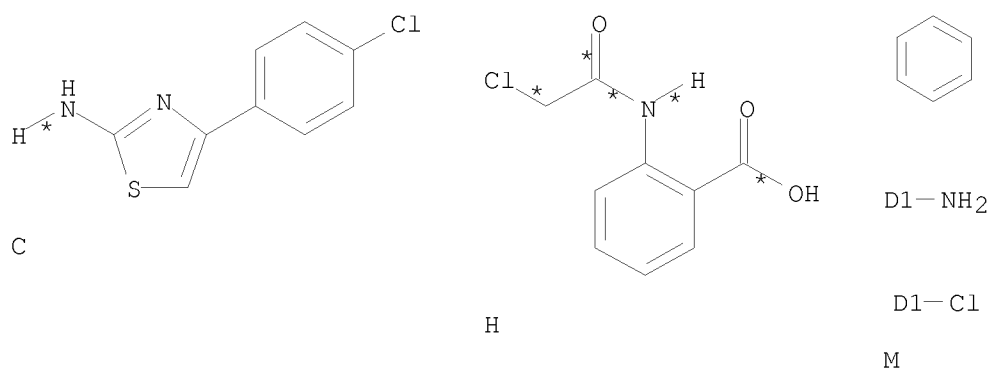
RX(1) RCT A 99-91-2, B 62-56-6

10/ 562,112

RGT D 7726-95-6 Br2  
PRO C 2103-99-3  
SOL 64-17-5 EtOH  
CON overnight, reflux

RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K2CO3  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

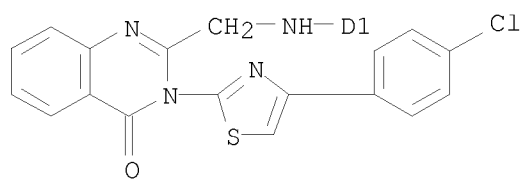
RX(16) OF 56 COMPOSED OF RX(3), RX(4)  
RX(16) C + H + M ==> N



2  
STEPS  
=>



D1-C1



N

RX(3) RCT C 2103-99-3, H 14422-49-2

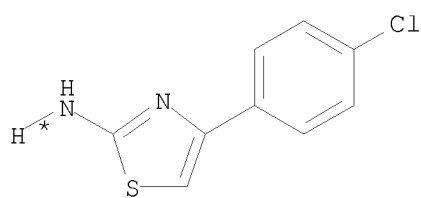
10/ 562,112

RGT L 584-08-7 K2CO3  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

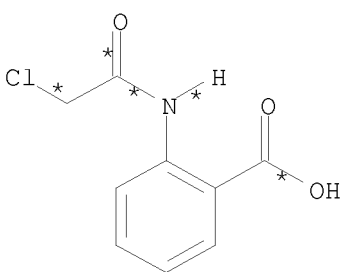
RX(4) RCT M 27134-26-5, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO N 934817-07-9  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(17) OF 56 COMPOSED OF RX(3), RX(5)

RX(17) C + H + P ==> Q



C



H



D1-NH2

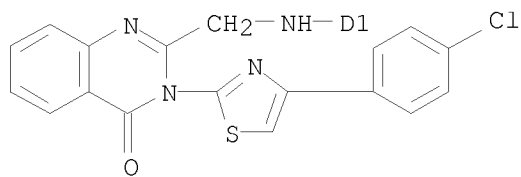
D1-F

P

2  
STEPS  
→



D1-F



Q

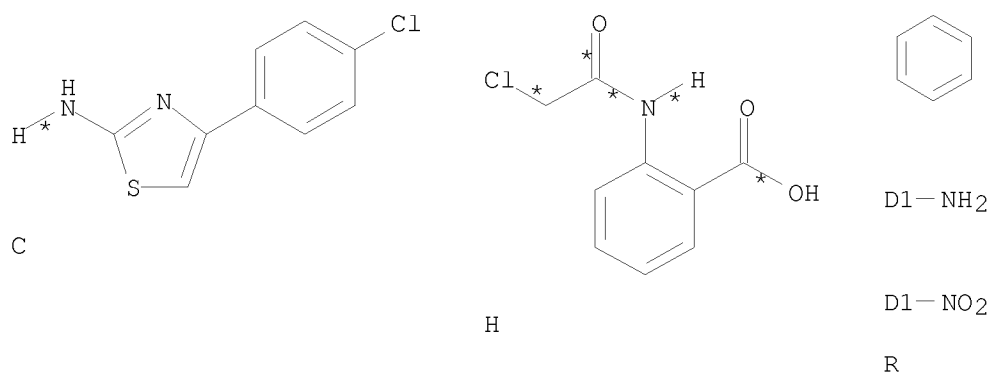
RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K2CO3

10/ 562,112

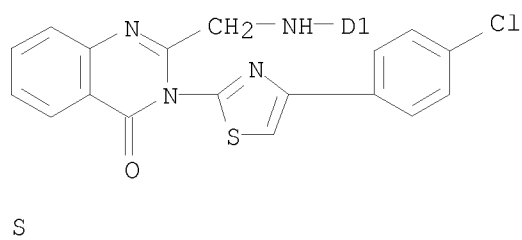
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

RX(5) RCT P 87686-42-8, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO Q 934817-08-0  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(18) OF 56 COMPOSED OF RX(3), RX(6)  
RX(18) C + H + R ==> S



D1-NO<sub>2</sub>



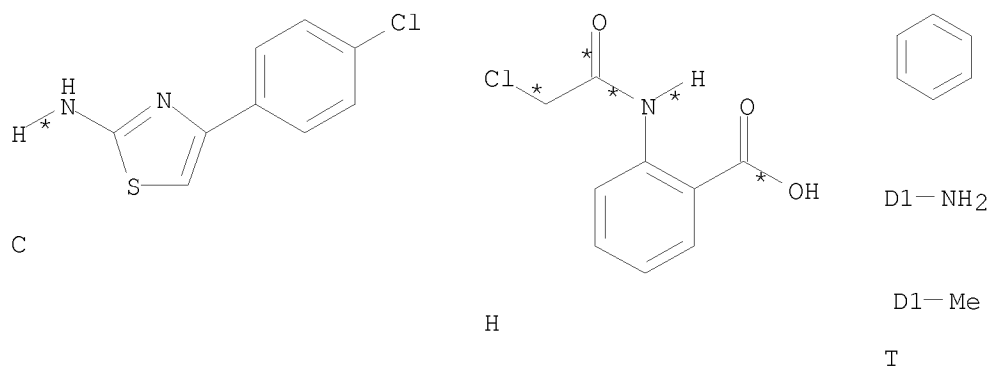
RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO K 870539-40-5

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SOL 64-17-5 EtOH  
CON 20 hours, reflux

RX(6) RCT R 29757-24-2, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO S 934817-09-1  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

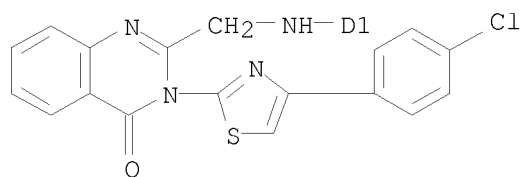
RX(19) OF 56 COMPOSED OF RX(3), RX(7)  
RX(19) C + H + T ==> U



2  
STEPS  
→



D1-Me



U

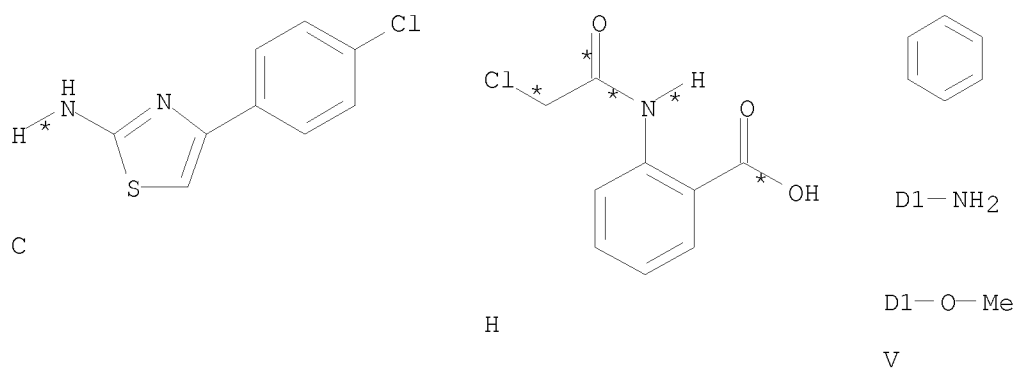
RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO K 870539-40-5  
SOL 64-17-5 EtOH

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CON 20 hours, reflux

RX(7) RCT T 26915-12-8, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO U 934817-10-4  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

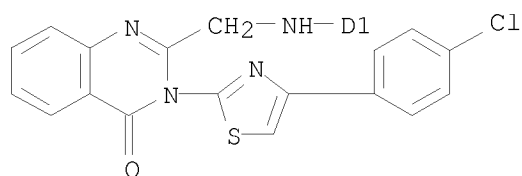
RX(20) OF 56 COMPOSED OF RX(3), RX(8)  
RX(20) C + H + V ==> W



2  
STEPS  
→



D1-O-Me



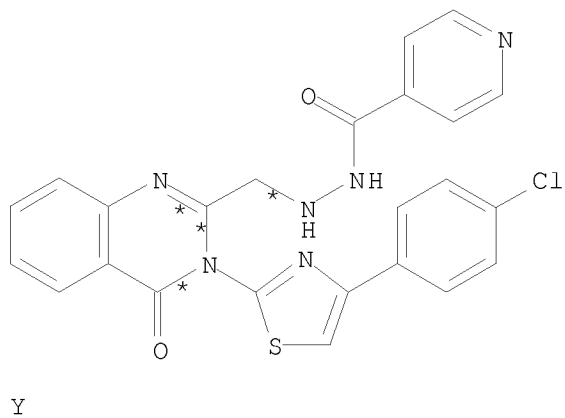
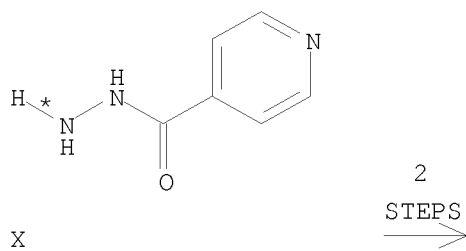
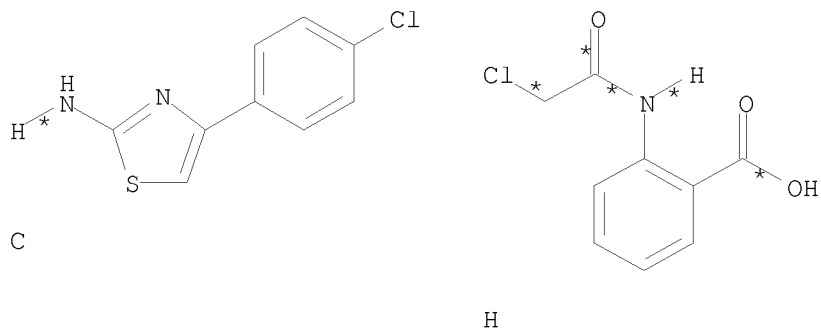
W

RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

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RX(8)        RCT   V 29191-52-4, K 870539-40-5  
              RGT   I 110-86-1 Pyridine  
              PRO   W 934817-11-5  
              SOL   108-24-7 Ac2O  
              CON   4 hours, reflux

RX(21) OF 56 COMPOSED OF RX(3), RX(9)  
RX(21)       C   +   H   +   X   ==>   Y



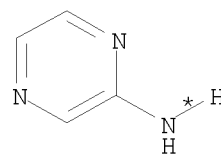
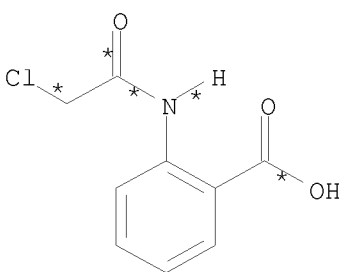
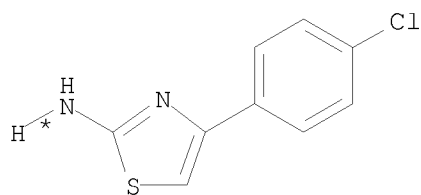
RX(3)        RCT   C 2103-99-3, H 14422-49-2  
              RGT   L 584-08-7 K2CO3  
              PRO   K 870539-40-5

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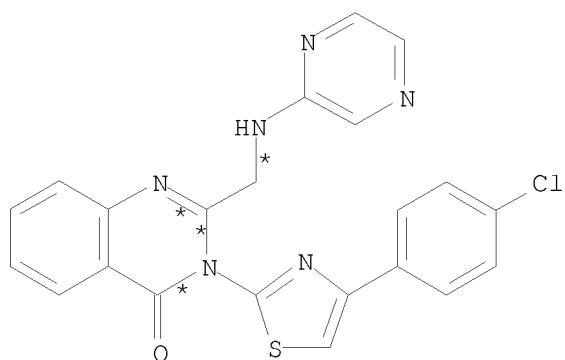
SOL 64-17-5 EtOH  
CON 20 hours, reflux

RX(9) RCT X 54-85-3, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO Y 934767-99-4  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(22) OF 56 COMPOSED OF RX(3), RX(10)  
RX(22) C + H + Z ==> AA



2  
STEPS  
→



RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K2CO3  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

RX(10) RCT Z 5049-61-6, K 870539-40-5  
RGT I 110-86-1 Pyridine

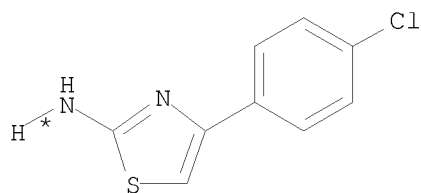


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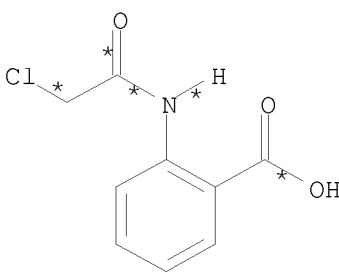
PRO AA 870539-37-0  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(23) OF 56 COMPOSED OF RX(3), RX(11)

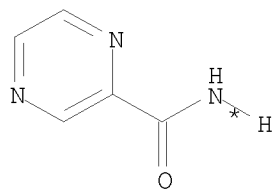
RX(23) C + H + AB ==> AC



C

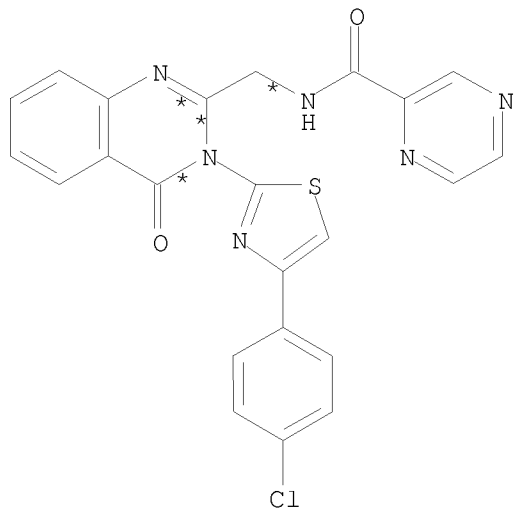


H



AB

2  
STEPS  
→



AC

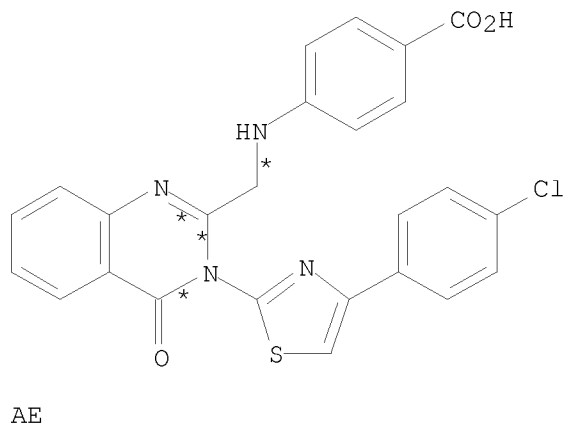
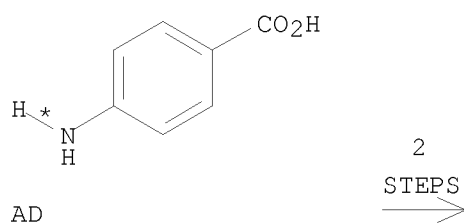
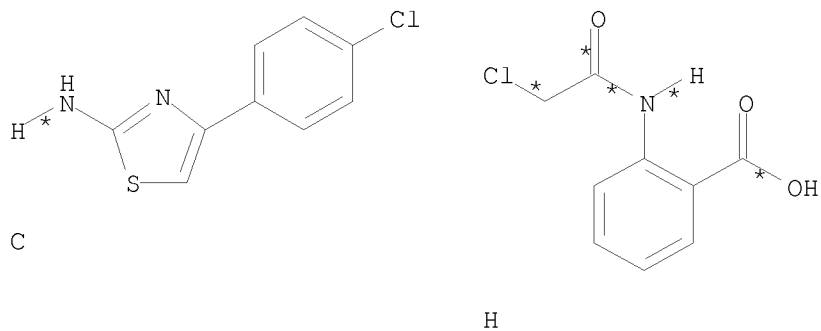
RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K2CO3

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PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

RX(11) RCT AB 98-96-4, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO AC 870539-38-1  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(24) OF 56 COMPOSED OF RX(3), RX(12)  
RX(24) C + H + AD ==> AE

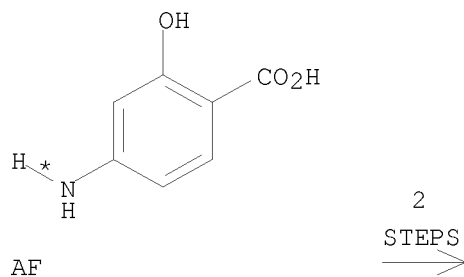
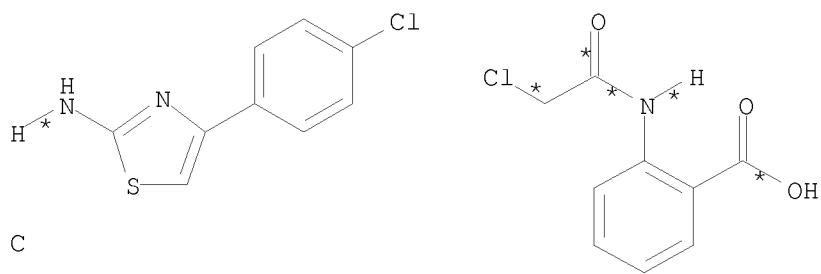


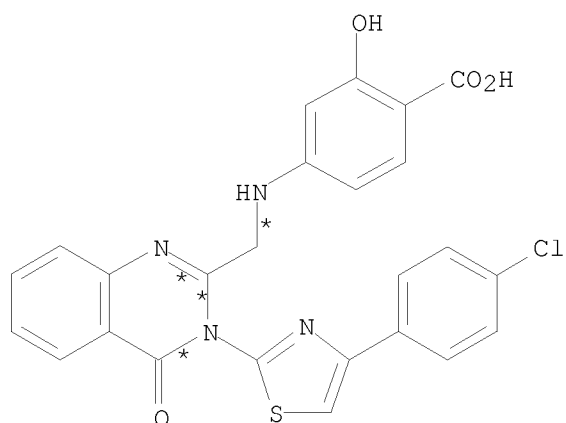
10/ 562,112

RX(3)        RCT   C 2103-99-3, H 14422-49-2  
              RGT   L 584-08-7 K2CO3  
              PRO   K 870539-40-5  
              SOL   64-17-5 EtOH  
              CON   20 hours, reflux

RX(12)      RCT   AD 150-13-0, K 870539-40-5  
              RGT   I 110-86-1 Pyridine  
              PRO   AE 934768-00-0  
              SOL   108-24-7 Ac2O  
              CON   4 hours, reflux

RX(25) OF 56 COMPOSED OF RX(3), RX(13)  
RX(25)      C + H + AF ==> AG



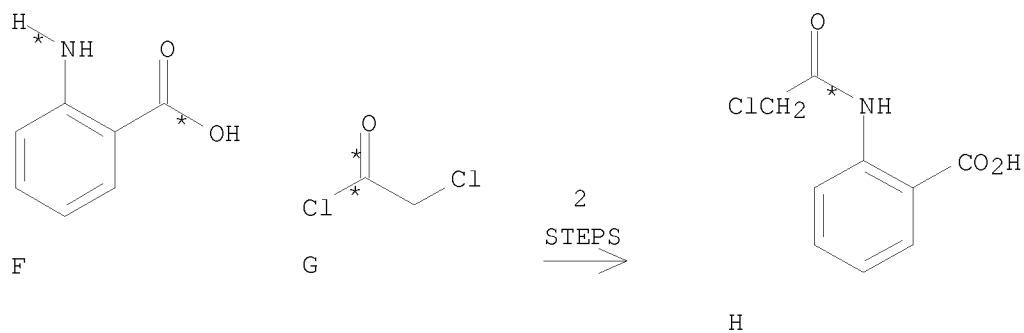


AG

RX(3)	RCT	C 2103-99-3, H 14422-49-2
	RGT	L 584-08-7 K2CO3
	PRO	K 870539-40-5
	SOL	64-17-5 EtOH
	CON	20 hours, reflux

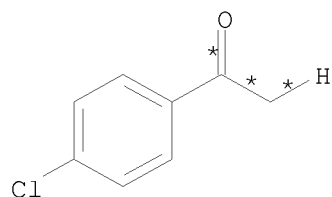
RX(13) RCT AF 65-49-6, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO AG 870539-39-2  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(26) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3)  
AND REACTION SEQUENCE RX(1), RX(3)

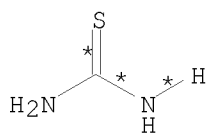
$$\begin{array}{rclcl} \dots F & + & G & \implies & H \dots \\ \dots A & + & B & + & H \implies K \end{array}$$


START NEXT REACTION SEQUENCE

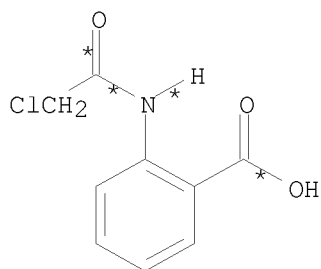
10/ 562,112



A

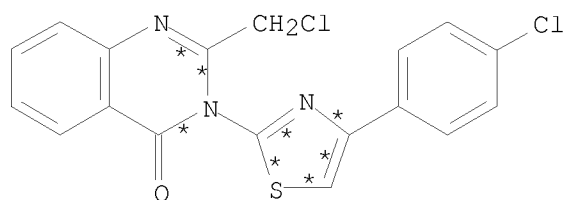


B



H

2  
STEPS  
→



K

YIELD 58%

RX(2)      RCT    F 118-92-3, G 79-04-9  
              RGT    I 110-86-1 Pyridine  
              PRO    H 14422-49-2  
              SOL    71-43-2 Benzene  
              CON    4 hours, reflux

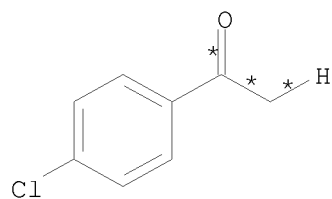
RX(1)      RCT    A 99-91-2, B 62-56-6  
              RGT    D 7726-95-6 Br2  
              PRO    C 2103-99-3  
              SOL    64-17-5 EtOH  
              CON    overnight, reflux

RX(3)      RCT    C 2103-99-3, H 14422-49-2  
              RGT    L 584-08-7 K2CO3  
              PRO    K 870539-40-5  
              SOL    64-17-5 EtOH  
              CON    20 hours, reflux

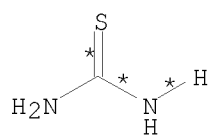
RX(27) OF 56 COMPOSED OF RX(1), RX(3), RX(4)

RX(27)      A + B + H + M ==> N

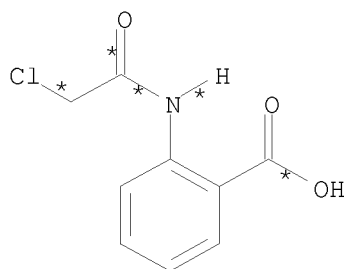
10/ 562,112



A



B



H



D1-NH<sub>2</sub>

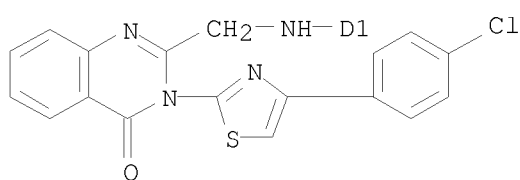


D1-Cl

D1-Cl

M

3  
STEPS



N

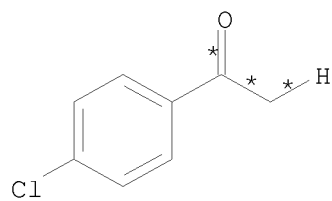
RX(1) RCT A 99-91-2, B 62-56-6  
RGT D 7726-95-6 Br<sub>2</sub>  
PRO C 2103-99-3  
SOL 64-17-5 EtOH  
CON overnight, reflux

RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

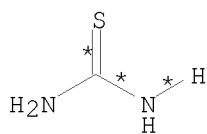
RX(4) RCT M 27134-26-5, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO N 934817-07-9  
SOL 108-24-7 Ac<sub>2</sub>O  
CON 4 hours, reflux

RX(28) OF 56 COMPOSED OF RX(1), RX(3), RX(5)  
RX(28) A + B + H + P ==> Q

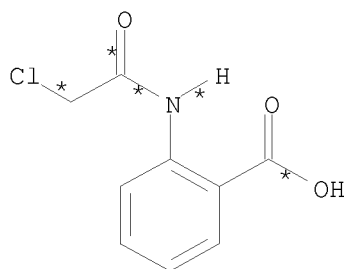
10/ 562,112



A



B



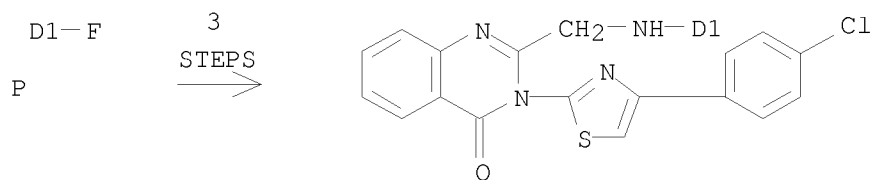
H



D1-NH<sub>2</sub>



D1-F



Q

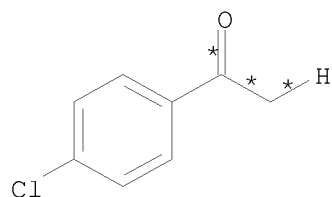
RX(1) RCT A 99-91-2, B 62-56-6  
RGT D 7726-95-6 Br<sub>2</sub>  
PRO C 2103-99-3  
SOL 64-17-5 EtOH  
CON overnight, reflux

RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

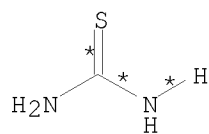
RX(5) RCT P 87686-42-8, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO Q 934817-08-0  
SOL 108-24-7 Ac<sub>2</sub>O  
CON 4 hours, reflux

RX(29) OF 56 COMPOSED OF RX(1), RX(3), RX(6)  
RX(29) A + B + H + R ==> S

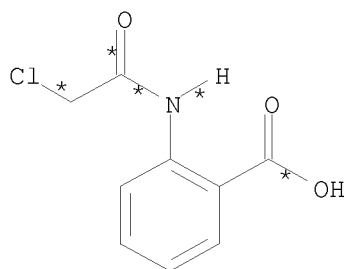
10/ 562,112



A



B



H



D1-NH<sub>2</sub>

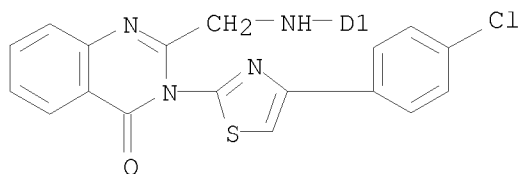


D1-NO<sub>2</sub>

D1-NO<sub>2</sub>

R

3  
STEPS  
→



S

RX(1) RCT A 99-91-2, B 62-56-6  
RGT D 7726-95-6 Br<sub>2</sub>  
PRO C 2103-99-3  
SOL 64-17-5 EtOH  
CON overnight, reflux

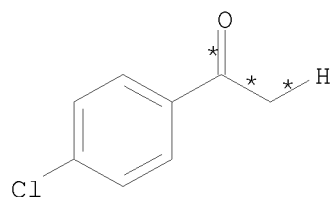
RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

RX(6) RCT R 29757-24-2, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO S 934817-09-1  
SOL 108-24-7 Ac<sub>2</sub>O  
CON 4 hours, reflux

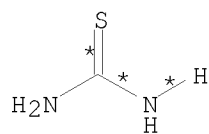
RX(30) OF 56 COMPOSED OF RX(1), RX(3), RX(7)  
RX(30) A + B + H + T ==> U



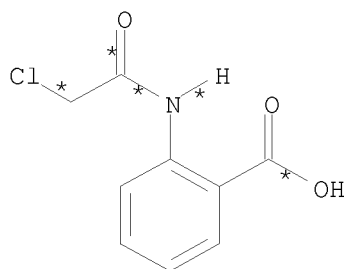
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A



B



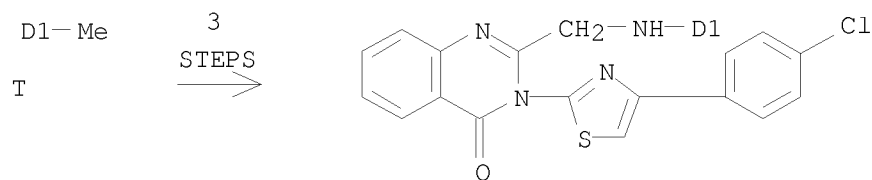
H



D1-NH<sub>2</sub>



D1-Me



U

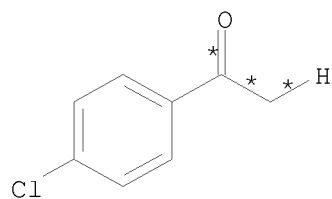
RX(1) RCT A 99-91-2, B 62-56-6  
RGT D 7726-95-6 Br<sub>2</sub>  
PRO C 2103-99-3  
SOL 64-17-5 EtOH  
CON overnight, reflux

RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

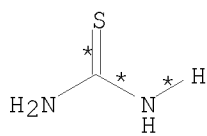
RX(7) RCT T 26915-12-8, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO U 934817-10-4  
SOL 108-24-7 Ac<sub>2</sub>O  
CON 4 hours, reflux

RX(31) OF 56 COMPOSED OF RX(1), RX(3), RX(8)  
RX(31) A + B + H + V ==> W

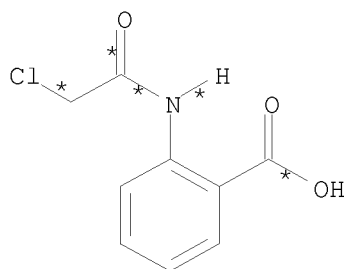
10/ 562,112



A



B



H



D1-NH<sub>2</sub>

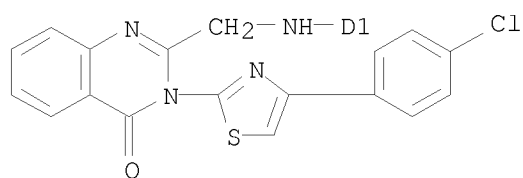


D1-O-Me

D1-O-Me

V

3  
STEPS  
→



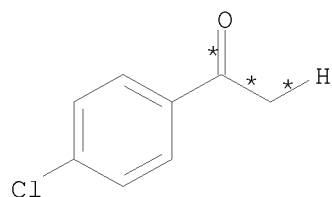
W

RX(1) RCT A 99-91-2, B 62-56-6  
RGT D 7726-95-6 Br<sub>2</sub>  
PRO C 2103-99-3  
SOL 64-17-5 EtOH  
CON overnight, reflux

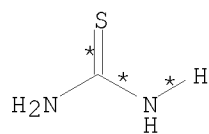
RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

RX(8) RCT V 29191-52-4, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO W 934817-11-5  
SOL 108-24-7 Ac<sub>2</sub>O  
CON 4 hours, reflux

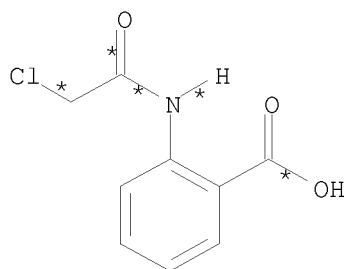
RX(32) OF 56 COMPOSED OF RX(1), RX(3), RX(9)  
RX(32) A + B + H + X ==> Y



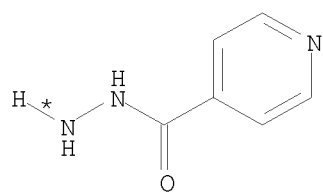
A



B

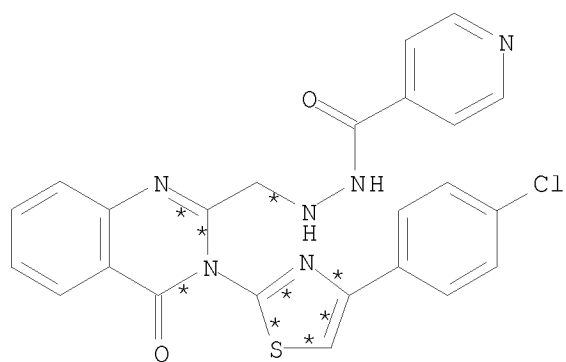


H



X

3  
STEPS  
→



Y

RX(1) RCT A 99-91-2, B 62-56-6  
 RGT D 7726-95-6 Br<sub>2</sub>  
 PRO C 2103-99-3  
 SOL 64-17-5 EtOH  
 CON overnight, reflux

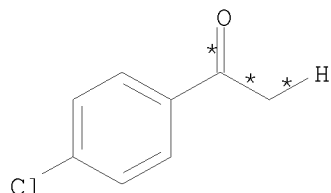
RX(3) RCT C 2103-99-3, H 14422-49-2  
 RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO K 870539-40-5  
 SOL 64-17-5 EtOH  
 CON 20 hours, reflux

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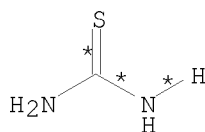
RX(9) RCT X 54-85-3, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO Y 934767-99-4  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(33) OF 56 COMPOSED OF RX(1), RX(3), RX(10)

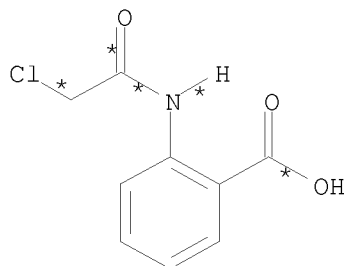
RX(33) A + B + H + Z ==> AA



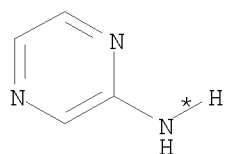
A



B

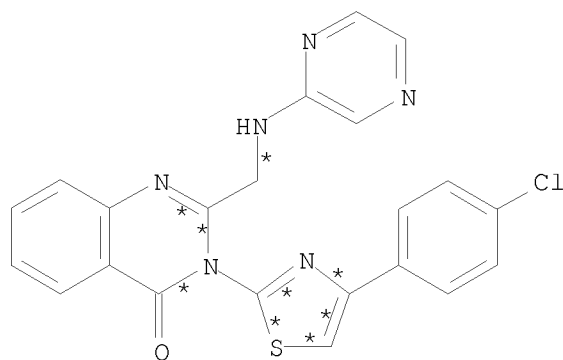


H



Z

3  
STEPS  
→



AA

RX(1) RCT A 99-91-2, B 62-56-6  
RGT D 7726-95-6 Br<sub>2</sub>  
PRO C 2103-99-3  
SOL 64-17-5 EtOH  
CON overnight, reflux

RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

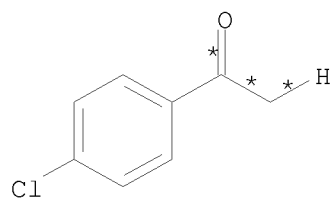
RX(10) RCT Z 5049-61-6, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO AA 870539-37-0  
SOL 108-24-7 Ac<sub>2</sub>O

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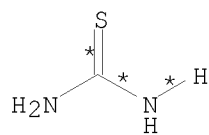
CON 4 hours, reflux

RX(34) OF 56 COMPOSED OF RX(1), RX(3), RX(11)

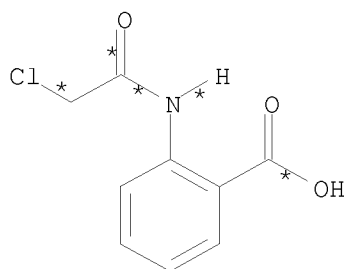
RX(34) A + B + H + AB ==> AC



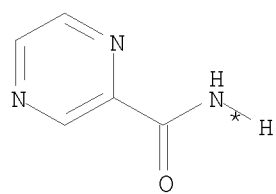
A



B

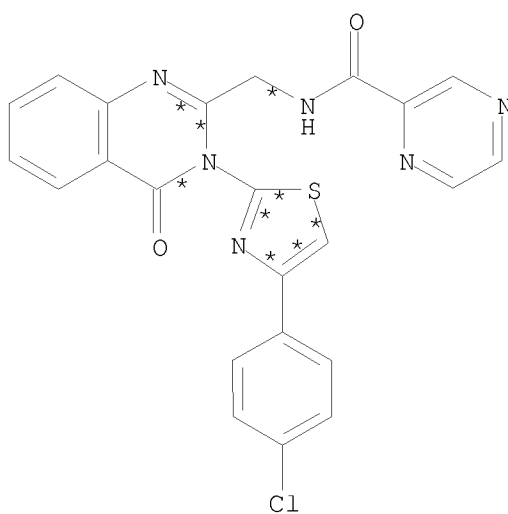


H



AB

3  
STEPS  
→



AC

RX(1) RCT A 99-91-2, B 62-56-6  
RGT D 7726-95-6 Br<sub>2</sub>  
PRO C 2103-99-3  
SOL 64-17-5 EtOH  
CON overnight, reflux

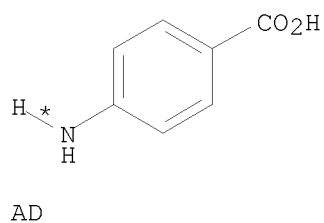
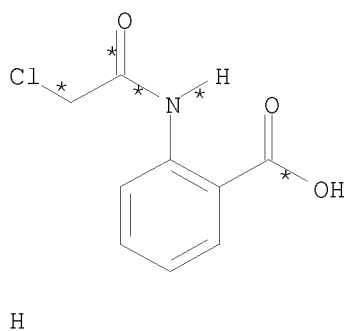
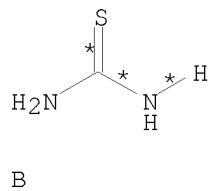
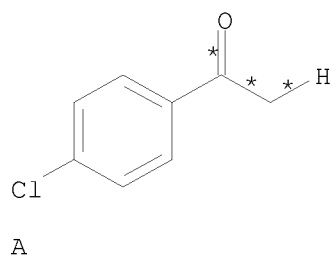
RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

RX(11) RCT AB 98-96-4, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO AC 870539-38-1

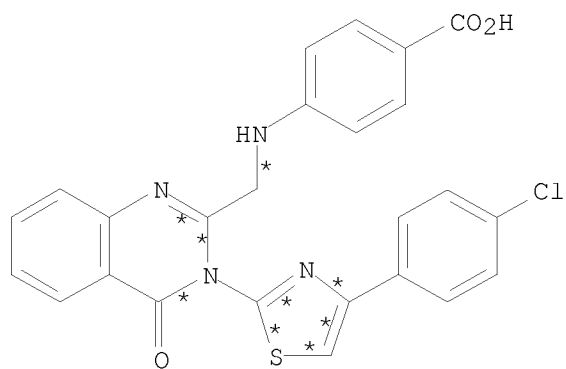
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SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(35) OF 56 COMPOSED OF RX(1), RX(3), RX(12)  
RX(35) A + B + H + AD ==> AE



3  
STEPS  
→



RX(1) RCT A 99-91-2, B 62-56-6  
RGT D 7726-95-6 Br2  
PRO C 2103-99-3  
SOL 64-17-5 EtOH  
CON overnight, reflux

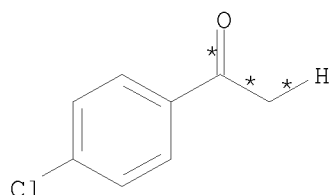
RX(3) RCT C 2103-99-3, H 14422-49-2

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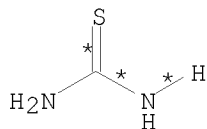
RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

RX(12) RCT AD 150-13-0, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO AE 934768-00-0  
SOL 108-24-7 Ac<sub>2</sub>O  
CON 4 hours, reflux

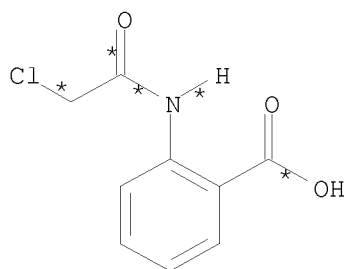
RX(36) OF 56 COMPOSED OF RX(1), RX(3), RX(13)  
RX(36) A + B + H + AF ==> AG



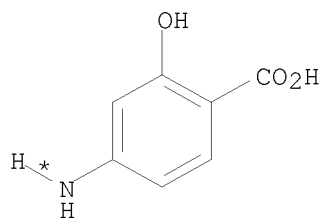
A



B

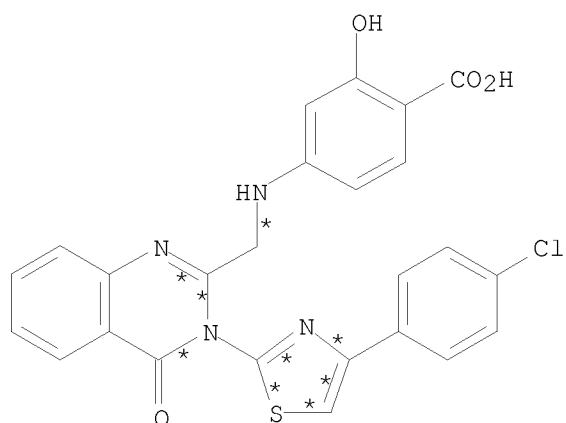


H



AF

3  
STEPS  
→



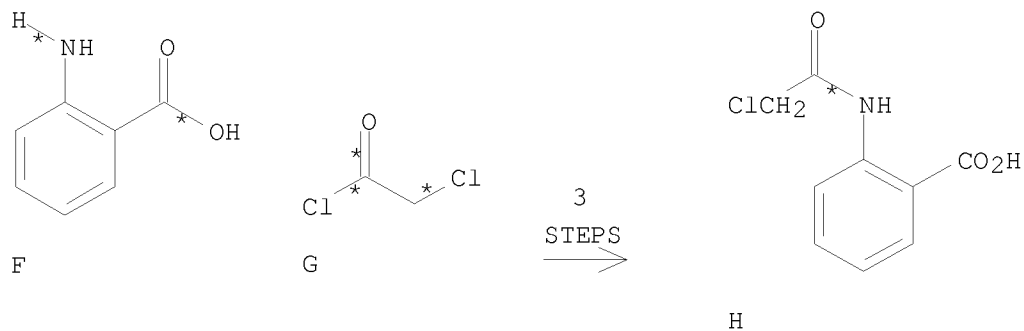
AG

RX(1)	RCT	A 99-91-2, B 62-56-6
	RGT	D 7726-95-6 Br2
	PRO	C 2103-99-3
	SOL	64-17-5 EtOH
	CON	overnight, reflux

RX(3)	RCT	C 2103-99-3, H 14422-49-2
	RGT	L 584-08-7 K2CO3
	PRO	K 870539-40-5
	SOL	64-17-5 EtOH
	CON	20 hours, reflux

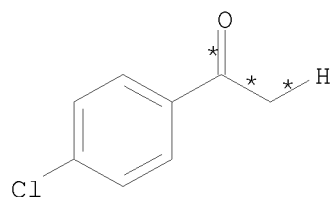
RX(13)      RCT    AF 65-49-6, K 870539-40-5  
              RGT    I 110-86-1 Pyridine  
              PRO    AG 870539-39-2  
              SOL    108-24-7 Ac2O  
              CON    4 hours, reflux

RX(47) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(4)  
AND REACTION SEQUENCE RX(1), RX(3), RX(4)

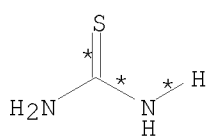
$$\begin{array}{rcll} \dots F & + & G & \implies H \dots \\ \dots A & + & B & + H + M \implies N \end{array}$$


START NEXT REACTION SEQUENCE

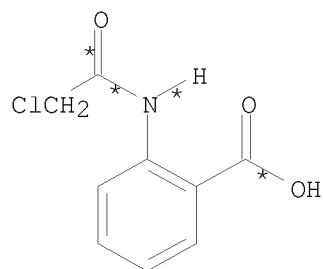




A



B



H

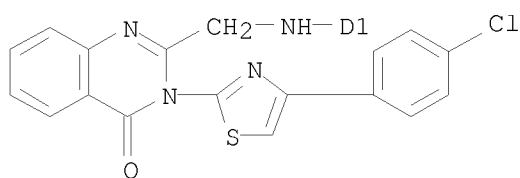
D1-NH<sub>2</sub>

D1-Cl

D1-Cl

M

3  
STEPS



N

RX(2) RCT F 118-92-3, G 79-04-9  
 RGT I 110-86-1 Pyridine  
 PRO H 14422-49-2  
 SOL 71-43-2 Benzene  
 CON 4 hours, reflux

RX(1) RCT A 99-91-2, B 62-56-6  
 RGT D 7726-95-6 Br<sub>2</sub>  
 PRO C 2103-99-3  
 SOL 64-17-5 EtOH  
 CON overnight, reflux

RX(3) RCT C 2103-99-3, H 14422-49-2  
 RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO K 870539-40-5  
 SOL 64-17-5 EtOH  
 CON 20 hours, reflux

RX(4) RCT M 27134-26-5, K 870539-40-5  
 RGT I 110-86-1 Pyridine  
 PRO N 934817-07-9  
 SOL 108-24-7 Ac<sub>2</sub>O

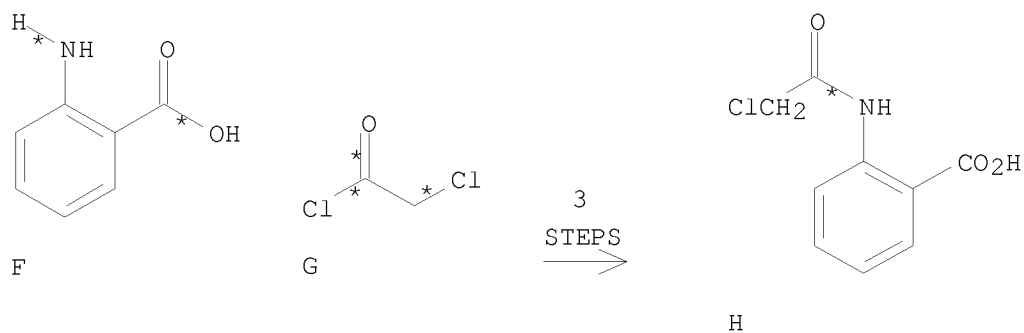
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CON 4 hours, reflux

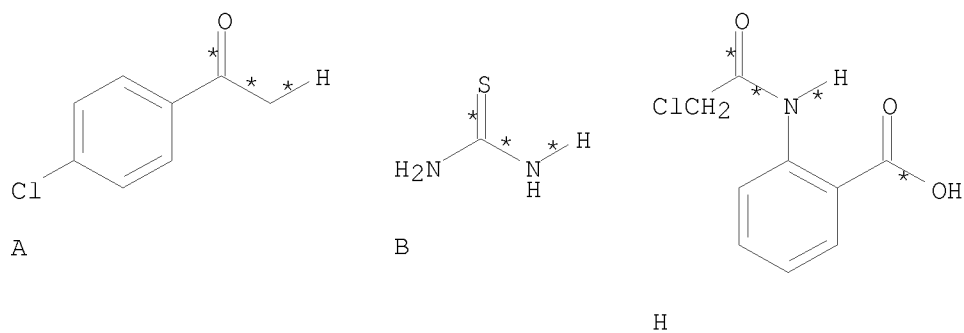
RX(48) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(5)  
AND REACTION SEQUENCE RX(1), RX(3), RX(5)

...F + G ==> H...

...A + B + H + P ==> Q



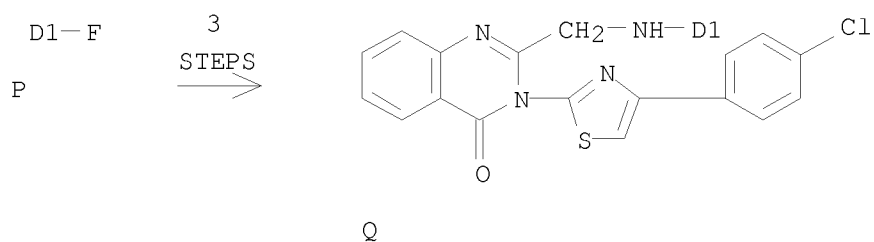
START NEXT REACTION SEQUENCE



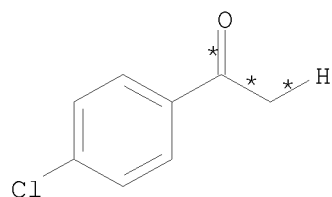
D1-NH<sub>2</sub>



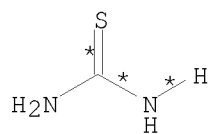
D1-F



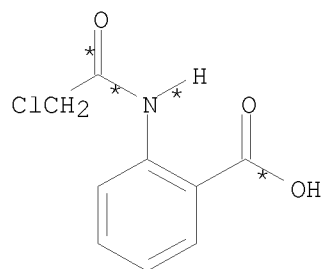




A



B

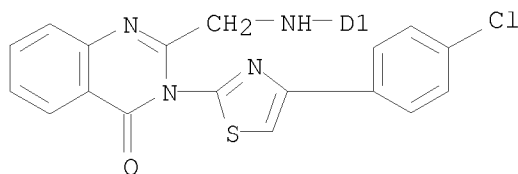


H

D1-NH<sub>2</sub>D1-NO<sub>2</sub>D1-NO<sub>2</sub>

R

3  
STEPS  
→



S

RX(2) RCT F 118-92-3, G 79-04-9  
RGT I 110-86-1 Pyridine  
PRO H 14422-49-2  
SOL 71-43-2 Benzene  
CON 4 hours, reflux

RX(1) RCT A 99-91-2, B 62-56-6  
RGT D 7726-95-6 Br<sub>2</sub>  
PRO C 2103-99-3  
SOL 64-17-5 EtOH  
CON overnight, reflux

RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

RX(6) RCT R 29757-24-2, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO S 934817-09-1  
SOL 108-24-7 Ac<sub>2</sub>O

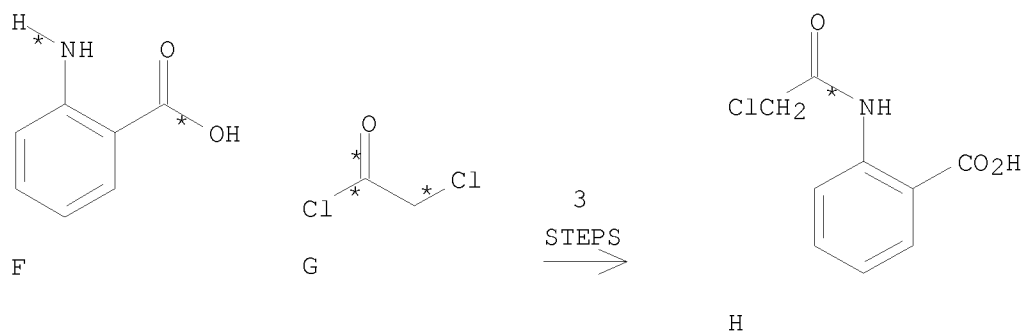
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CON 4 hours, reflux

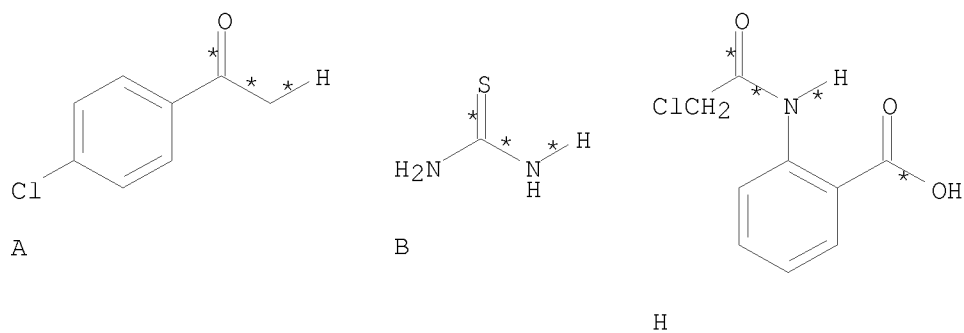
RX(50) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(7)  
AND REACTION SEQUENCE RX(1), RX(3), RX(7)

...F + G ==> H...

...A + B + H + T ==> U



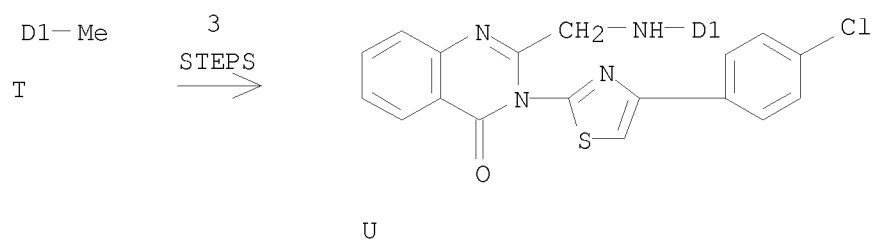
START NEXT REACTION SEQUENCE



D1-NH<sub>2</sub>



D1-Me



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RX(2) RCT F 118-92-3, G 79-04-9  
RGT I 110-86-1 Pyridine  
PRO H 14422-49-2  
SOL 71-43-2 Benzene  
CON 4 hours, reflux

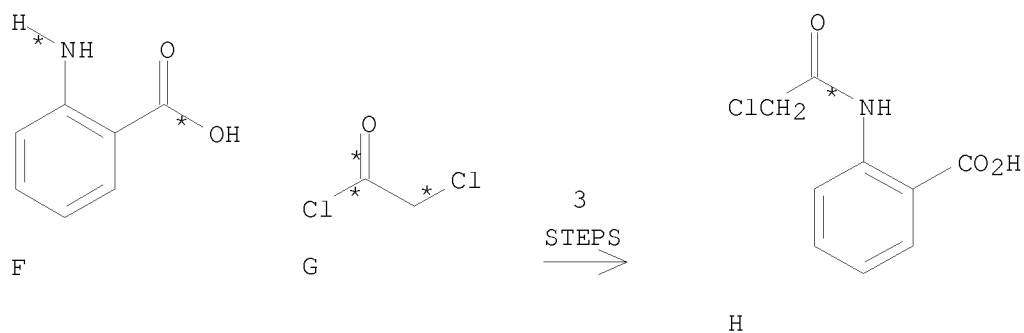
RX(1) RCT A 99-91-2, B 62-56-6  
RGT D 7726-95-6 Br2  
PRO C 2103-99-3  
SOL 64-17-5 EtOH  
CON overnight, reflux

RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K2CO3  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

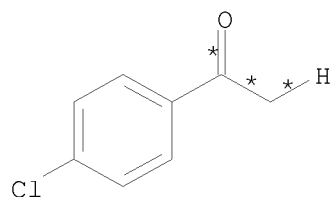
RX(7) RCT T 26915-12-8, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO U 934817-10-4  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

RX(51) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(8)  
AND REACTION SEQUENCE RX(1), RX(3), RX(8)

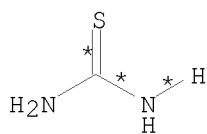
...F + G ==> H...  
...A + B + H + V ==> W



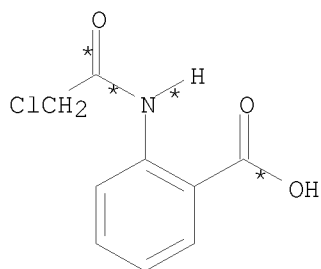
START NEXT REACTION SEQUENCE



A



B



H

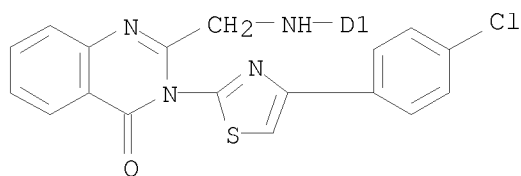
D1-NH<sub>2</sub>

D1-O-Me

D1-O-Me

V

3  
STEPS  
→



W

RX(2) RCT F 118-92-3, G 79-04-9  
RGT I 110-86-1 Pyridine  
PRO H 14422-49-2  
SOL 71-43-2 Benzene  
CON 4 hours, reflux

RX(1) RCT A 99-91-2, B 62-56-6  
RGT D 7726-95-6 Br<sub>2</sub>  
PRO C 2103-99-3  
SOL 64-17-5 EtOH  
CON overnight, reflux

RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

RX(8) RCT V 29191-52-4, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO W 934817-11-5  
SOL 108-24-7 Ac<sub>2</sub>O

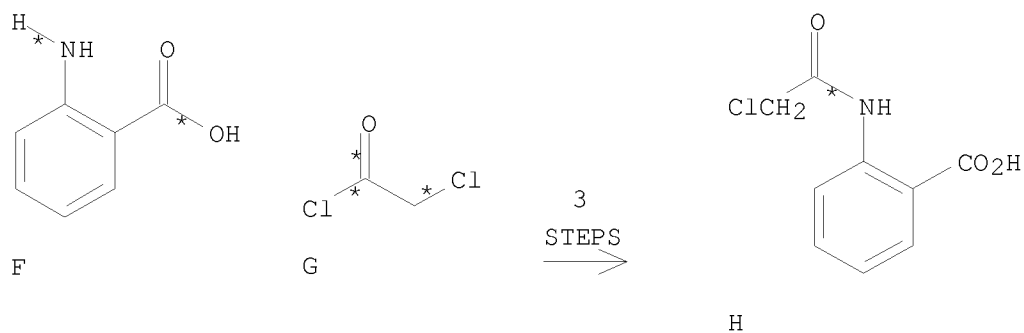
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CON 4 hours, reflux

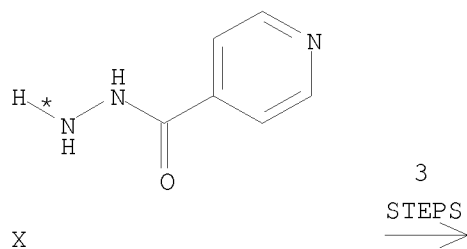
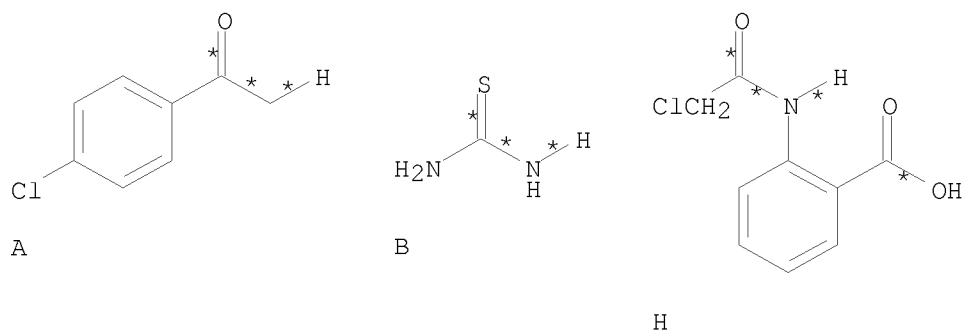
RX(52) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(9)  
AND REACTION SEQUENCE RX(1), RX(3), RX(9)

...F + G ==> H...

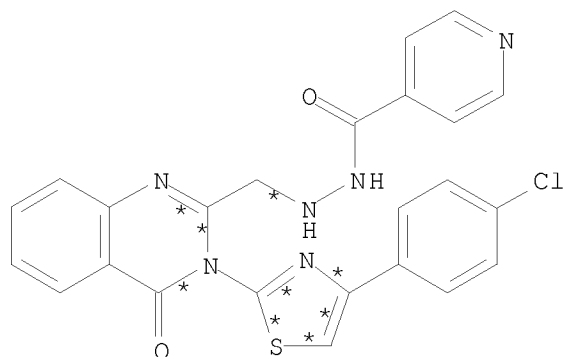
...A + B + H + X ==> Y



START NEXT REACTION SEQUENCE







Y

RX(2) RCT F 118-92-3, G 79-04-9  
 RGT I 110-86-1 Pyridine  
 PRO H 14422-49-2  
 SOL 71-43-2 Benzene  
 CON 4 hours, reflux

RX(1) RCT A 99-91-2, B 62-56-6  
 RGT D 7726-95-6 Br<sub>2</sub>  
 PRO C 2103-99-3  
 SOL 64-17-5 EtOH  
 CON overnight, reflux

RX(3) RCT C 2103-99-3, H 14422-49-2  
 RGT L 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO K 870539-40-5  
 SOL 64-17-5 EtOH  
 CON 20 hours, reflux

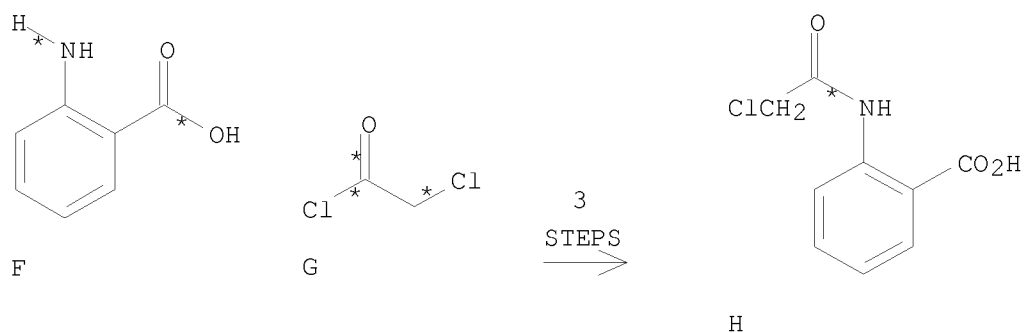
RX(9) RCT X 54-85-3, K 870539-40-5  
 RGT I 110-86-1 Pyridine  
 PRO Y 934767-99-4  
 SOL 108-24-7 Ac<sub>2</sub>O  
 CON 4 hours, reflux

RX(53) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(10)  
 AND REACTION SEQUENCE RX(1), RX(3), RX(10)

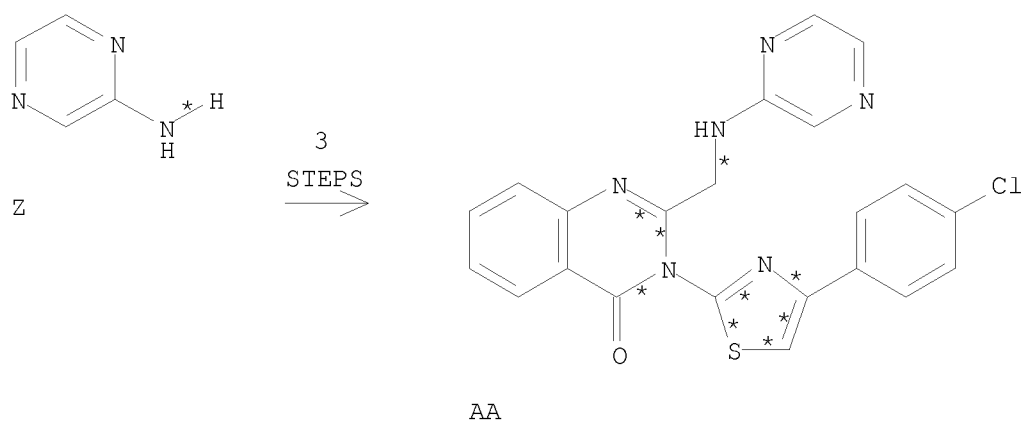
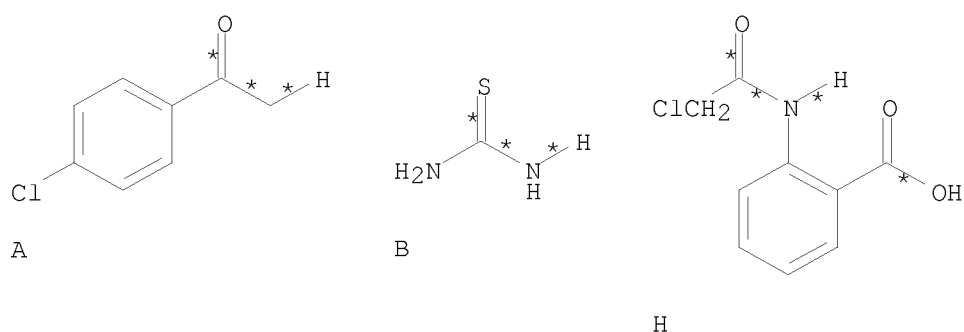
...F + G ==> H...

...A + B + H + Z ==> AA

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START NEXT REACTION SEQUENCE



RX(2)      RCT    F 118-92-3, G 79-04-9  
               RGT    I 110-86-1 Pyridine  
               PRO    H 14422-49-2  
               SOL    71-43-2 Benzene  
               CON    4 hours, reflux

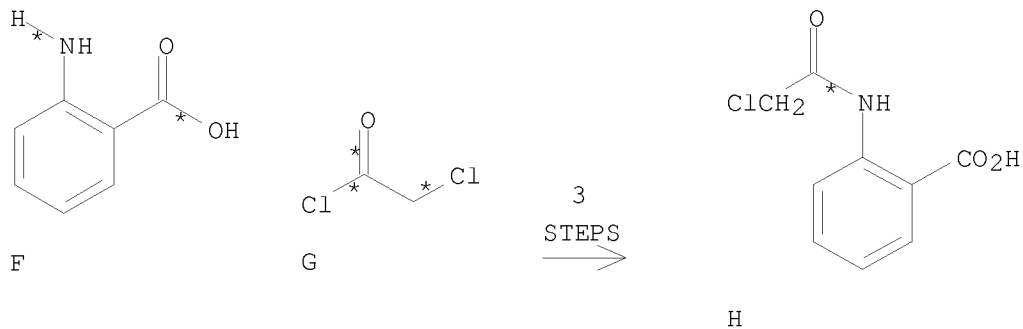
RX(1)      RCT    A 99-91-2, B 62-56-6  
               RGT    D 7726-95-6 Br<sub>2</sub>  
               PRO    C 2103-99-3  
               SOL    64-17-5 EtOH  
               CON    overnight, reflux

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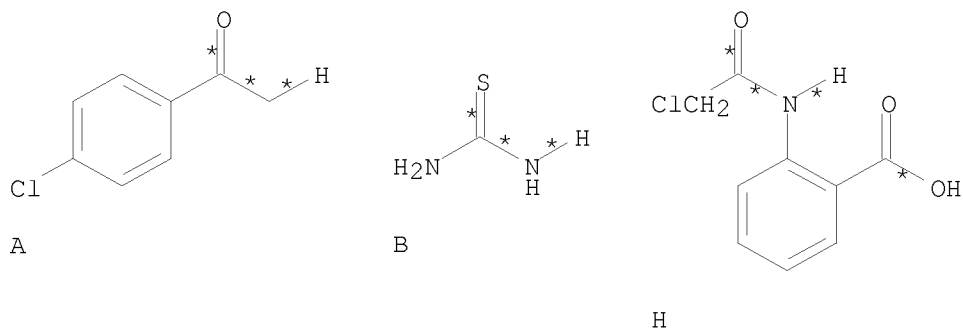
RX(3)	RCT	C 2103-99-3, H 14422-49-2
	RGT	L 584-08-7 K2CO3
	PRO	K 870539-40-5
	SOL	64-17-5 EtOH
	CON	20 hours, reflux

RX(10) RCT Z 5049-61-6, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO AA 870539-37-0  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

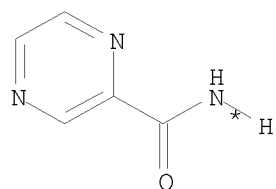
RX(54) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(11)  
AND REACTION SEQUENCE RX(1), RX(3), RX(11)

$$\dots F + G \implies H \dots$$
$$\dots A + B + H + AB \implies AC$$


START NEXT REACTION SEQUENCE



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AB

3  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT F 118-92-3, G 79-04-9  
RGT I 110-86-1 Pyridine  
PRO H 14422-49-2  
SOL 71-43-2 Benzene  
CON 4 hours, reflux

RX(1) RCT A 99-91-2, B 62-56-6  
RGT D 7726-95-6 Br2  
PRO C 2103-99-3  
SOL 64-17-5 EtOH  
CON overnight, reflux

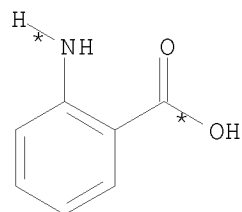
RX(3) RCT C 2103-99-3, H 14422-49-2  
RGT L 584-08-7 K2CO3  
PRO K 870539-40-5  
SOL 64-17-5 EtOH  
CON 20 hours, reflux

RX(11) RCT AB 98-96-4, K 870539-40-5  
RGT I 110-86-1 Pyridine  
PRO AC 870539-38-1  
SOL 108-24-7 Ac2O  
CON 4 hours, reflux

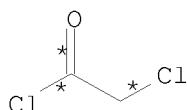
RX(55) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(12)  
AND REACTION SEQUENCE RX(1), RX(3), RX(12)

...F + G ==> H...

...A + B + H + AD ==> AE



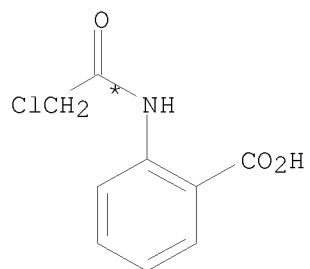
F



G

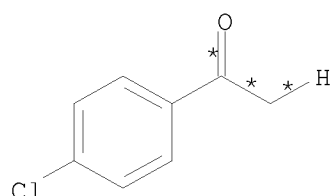
3  
STEPS  
→

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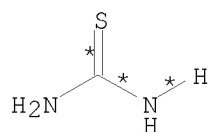


H

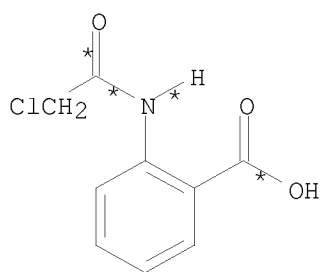
START NEXT REACTION SEQUENCE



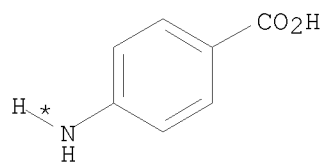
A



B

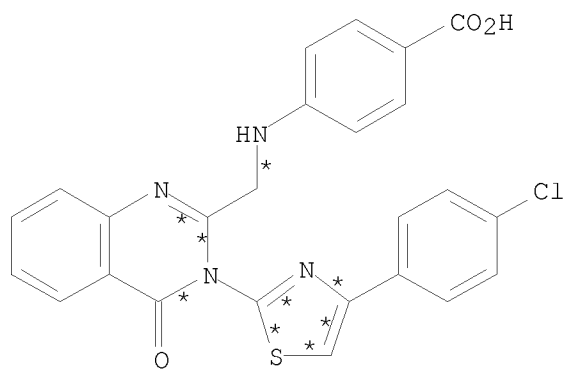


H



AD

3  
STEPS  
→



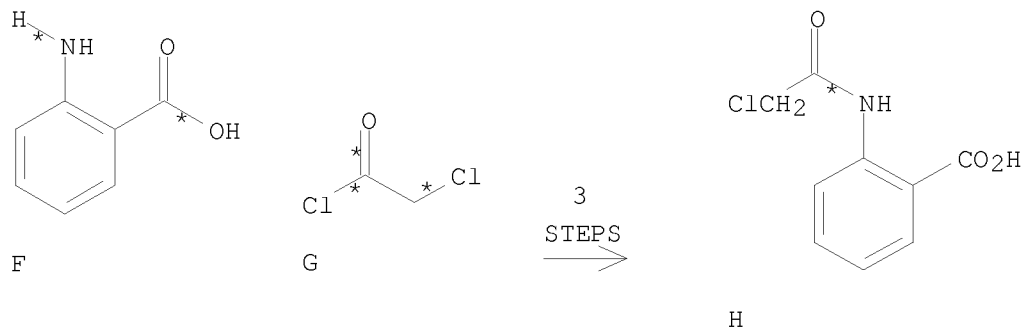
AE

RX(2)      RCT    F 118-92-3, G 79-04-9  
              RGT    I 110-86-1 Pyridine  
              PRO    H 14422-49-2  
              SOL    71-43-2 Benzene  
              CON    4 hours, reflux  
  
 RX(1)      RCT    A 99-91-2, B 62-56-6  
              RGT    D 7726-95-6 Br2  
              PRO    C 2103-99-3  
              SOL    64-17-5 EtOH  
              CON    overnight, reflux  
  
 RX(3)      RCT    C 2103-99-3, H 14422-49-2  
              RGT    L 584-08-7 K2CO3  
              PRO    K 870539-40-5  
              SOL    64-17-5 EtOH  
              CON    20 hours, reflux  
  
 RX(12)     RCT    AD 150-13-0, K 870539-40-5  
              RGT    I 110-86-1 Pyridine  
              PRO    AE 934768-00-0  
              SOL    108-24-7 Ac2O  
              CON    4 hours, reflux

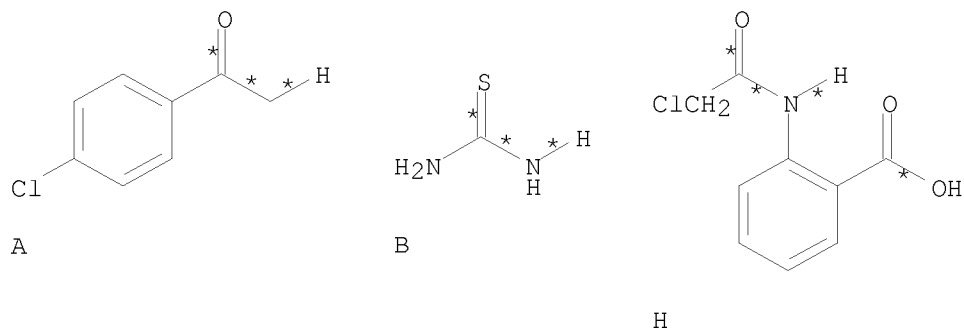
RX(56) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(13)  
 AND REACTION SEQUENCE RX(1), RX(3), RX(13)

...F + G ==> H...

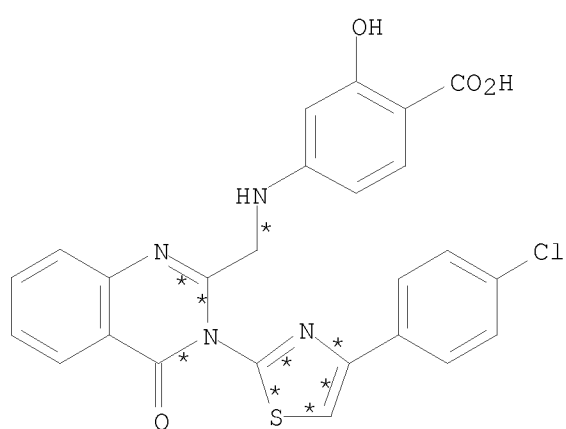
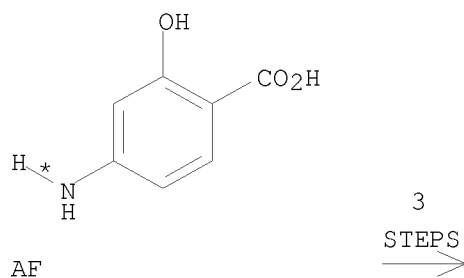
...A + B + H + AF ==> AG



START NEXT REACTION SEQUENCE



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AG

RX(2)	RCT	F 118-92-3, G 79-04-9
	RGT	I 110-86-1 Pyridine
	PRO	H 14422-49-2
	SOL	71-43-2 Benzene
	CON	4 hours, reflux
RX(1)	RCT	A 99-91-2, B 62-56-6
	RGT	D 7726-95-6 Br <sub>2</sub>
	PRO	C 2103-99-3
	SOL	64-17-5 EtOH
	CON	overnight, reflux
RX(3)	RCT	C 2103-99-3, H 14422-49-2
	RGT	L 584-08-7 K <sub>2</sub> CO <sub>3</sub>
	PRO	K 870539-40-5
	SOL	64-17-5 EtOH
	CON	20 hours, reflux
RX(13)	RCT	AF 65-49-6, K 870539-40-5
	RGT	I 110-86-1 Pyridine
	PRO	AG 870539-39-2
	SOL	108-24-7 Ac <sub>2</sub> O
	CON	4 hours, reflux

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 24 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 146:421942 CASREACT

TITLE: Synthesis and behavior of  
2-carboxyvinyl-6,8-dibromo-4H-3,1-benzoxazin-4-one  
towards nitrogen, carbon and sulphur nucleophiles

AUTHOR(S): El-Hashash, M. A.; Abdel-Rahman, T. M.; El-Badry, Y.  
A.

CORPORATE SOURCE: Faculty of Science, Ain Shams University, Cairo, Egypt

SOURCE: Indian Journal of Chemistry, Section B: Organic  
Chemistry Including Medicinal Chemistry (2006),  
45B(6), 1470-1477

CODEN: IJSBDB; ISSN: 0376-4699

PUBLISHER: National Institute of Science Communication and  
Information Resources

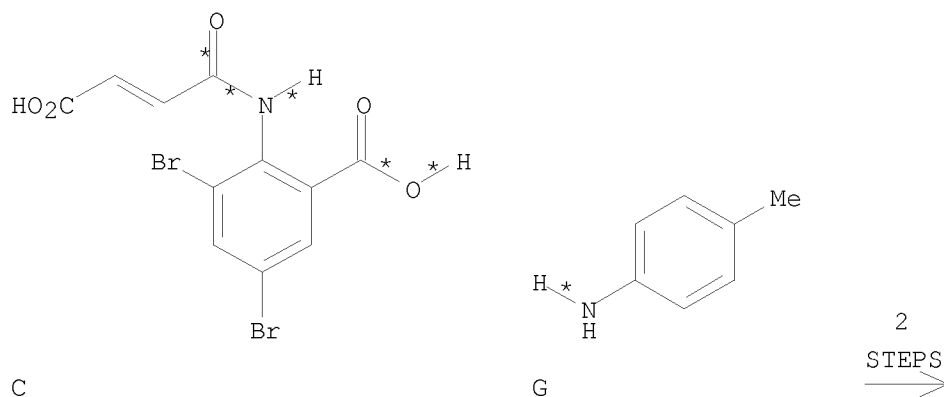
DOCUMENT TYPE: Journal

LANGUAGE: English

AB 3-(6,8-Dibromo-4-oxo-4H-3,1-benzoxazin-2-yl)-2-propenoic acid (I) is  
synthesized and allowed to react with some nitrogen nucleophiles namely,  
p-toluidine, hydroxylamine hydrochloride, ethanolamine, and glycine and  
affords 3-substituted quinazolinones, while with isobutylamine and  
benzylamine results benzamide derivs. Treatment of benzoxazinone I with  
o-phenylenediamine in different solvents under different conditions  
affords substituted benzamide and 3-substituted quinazolinone derivative

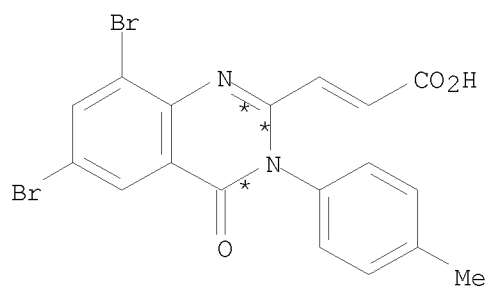
RX(33) OF 101 COMPOSED OF RX(2), RX(3)

RX(33) C + G ==> H





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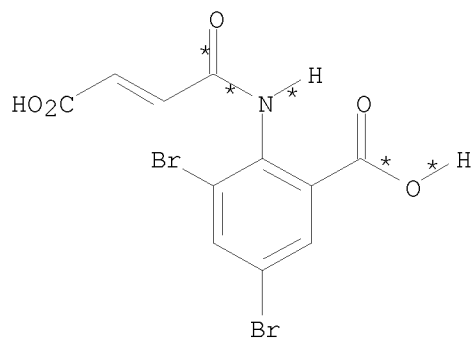


H  
YIELD 48%

RX(2)        RCT    C 934242-55-4  
              RGT    F 108-24-7 Ac2O  
              PRO    E 838868-31-8  
              SOL    108-24-7 Ac2O  
              CON    1 hour, heated

RX(3)        RCT    E 838868-31-8, G 106-49-0  
              PRO    H 934242-56-5  
              SOL    64-19-7 AcOH  
              CON    3 hours, reflux

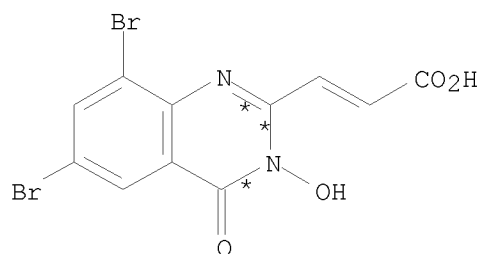
RX(34) OF 101 COMPOSED OF RX(2), RX(4)  
RX(34)        C    ==>    J



C

2  
STEPS  
→

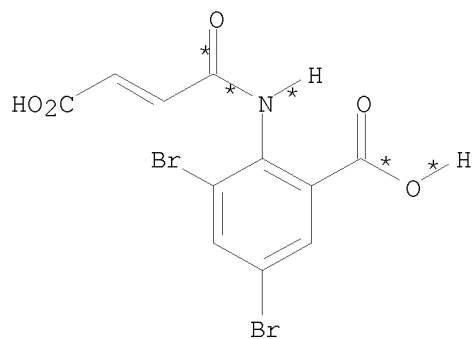
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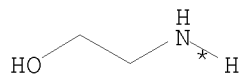
J  
YIELD 73%

RX(2)	RCT	C 934242-55-4
	RGT	F 108-24-7 Ac2O
	PRO	E 838868-31-8
	SOL	108-24-7 Ac2O
	CON	1 hour, heated
RX(4)	RCT	E 838868-31-8
	RGT	K 5470-11-1 H2NOH-HCl
	PRO	J 934242-57-6
	SOL	110-86-1 Pyridine
	CON	3 hours, reflux

RX(35) OF 101 COMPOSED OF RX(2), RX(5)  
RX(35) C + M ==> N



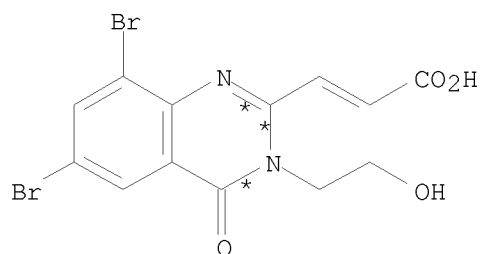
C



M

2  
STEPS  
→

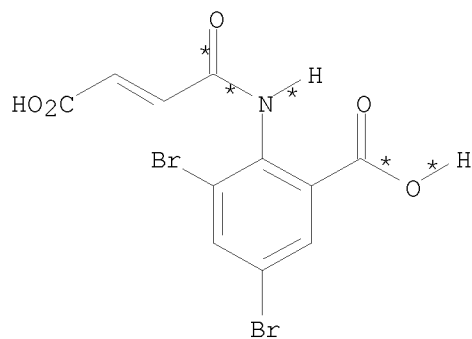
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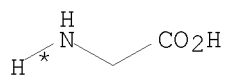
N  
YIELD 58%

RX(2)	RCT	C	934242-55-4
	RGT	F	108-24-7 Ac2O
	PRO	E	838868-31-8
	SOL		108-24-7 Ac2O
	CON		1 hour, heated
RX(5)	RCT	E	838868-31-8, M 141-43-5
	RGT	O	127-09-3 AcONa
	PRO	N	934242-58-7
	SOL		64-19-7 AcOH
	CON		3 hours, reflux

RX(36) OF 101 COMPOSED OF RX(2), RX(6)  
RX(36) C + P ==> Q



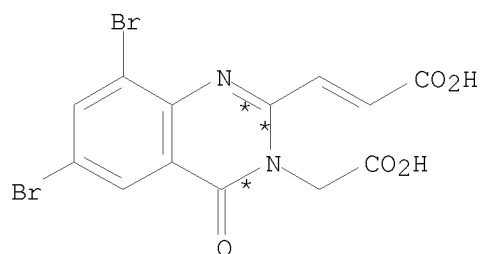
C



P

2  
STEPS  
→

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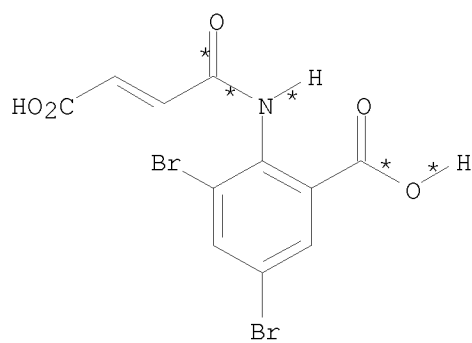


Q  
YIELD 44%

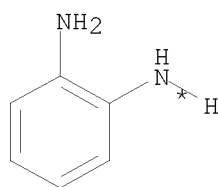
RX(2)      RCT   C 934242-55-4  
             RGT   F 108-24-7 Ac<sub>2</sub>O  
             PRO   E 838868-31-8  
             SOL   108-24-7 Ac<sub>2</sub>O  
             CON   1 hour, heated

RX(6)      RCT   E 838868-31-8, P 56-40-6  
             PRO   Q 934242-59-8  
             SOL   110-86-1 Pyridine  
             CON   8 hours, reflux

RX(40) OF 101 COMPOSED OF RX(2), RX(15)  
RX(40)      C + AJ ==> AL



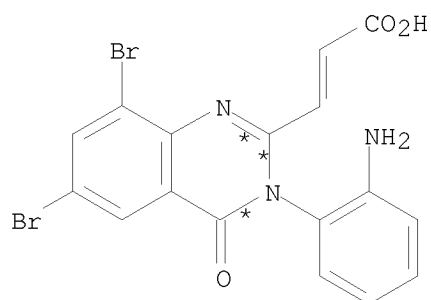
C



AJ

2  
STEPS  
→

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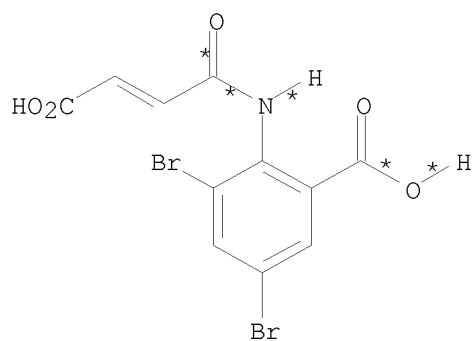


AL  
YIELD 56%

RX(2) RCT C 934242-55-4  
RGT F 108-24-7 Ac2O  
PRO E 838868-31-8  
SOL 108-24-7 Ac2O  
CON 1 hour, heated

RX(15) RCT E 838868-31-8, AJ 95-54-5  
RGT O 127-09-3 AcONa  
PRO AL 934242-68-9  
SOL 64-19-7 AcOH  
CON 2 hours, reflux

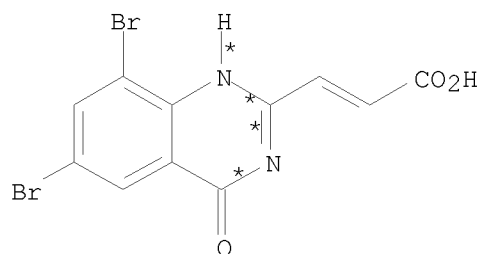
RX(41) OF 101 COMPOSED OF RX(2), RX(16)  
RX(41) C ==> AM



C

2  
STEPS  
→

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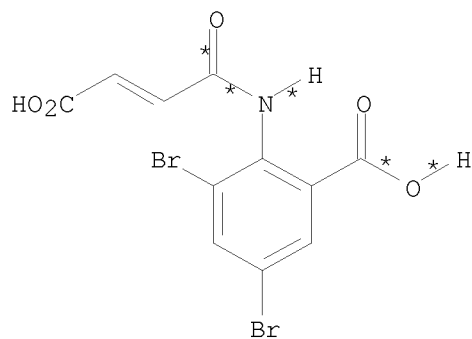


AM  
YIELD 65%

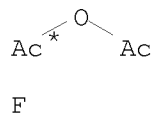
RX(2)      RCT    C 934242-55-4  
            RGT    F 108-24-7 Ac2O  
            PRO    E 838868-31-8  
            SOL    108-24-7 Ac2O  
            CON    1 hour, heated

RX(16)     RCT    E 838868-31-8  
            RGT    AN 75-12-7 Formamide  
            PRO    AM 934242-69-0  
            SOL    75-12-7 Formamide  
            CON    2 hours, reflux

RX(81) OF 101 COMPOSED OF RX(2), RX(4), RX(9)  
RX(81)      C    +    F    ==>    W

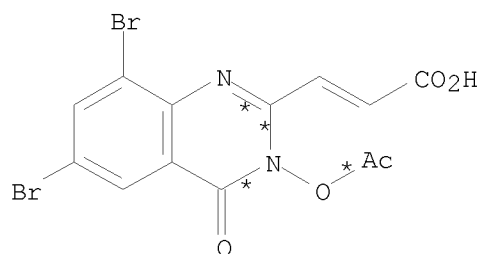


C



3  
STEPS  
→

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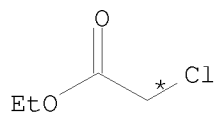
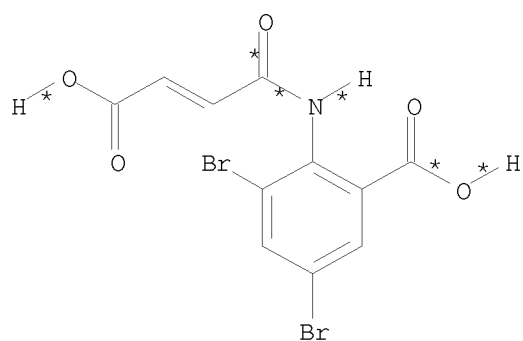
W  
YIELD 80%

RX(2)      RCT    C 934242-55-4  
             RGT    F 108-24-7 Ac2O  
             PRO    E 838868-31-8  
             SOL    108-24-7 Ac2O  
             CON    1 hour, heated

RX(4)      RCT    E 838868-31-8  
             RGT    K 5470-11-1 H2NOH-HCl  
             PRO    J 934242-57-6  
             SOL    110-86-1 Pyridine  
             CON    3 hours, reflux

RX(9)      RCT    J 934242-57-6, F 108-24-7  
             PRO    W 934242-62-3  
             SOL    108-24-7 Ac2O  
             CON    2 hours, reflux

RX(82) OF 101 COMPOSED OF RX(2), RX(4), RX(10)  
RX(82)      C    +    2 X    ==>    Y

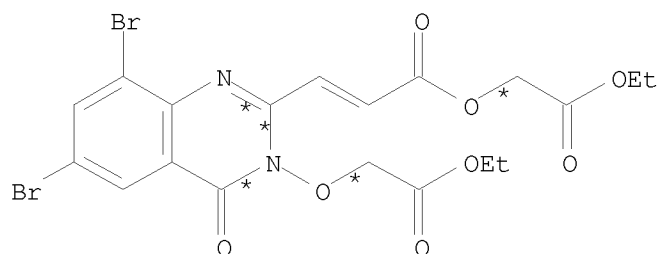


C

2 X

3  
STEPS  
→

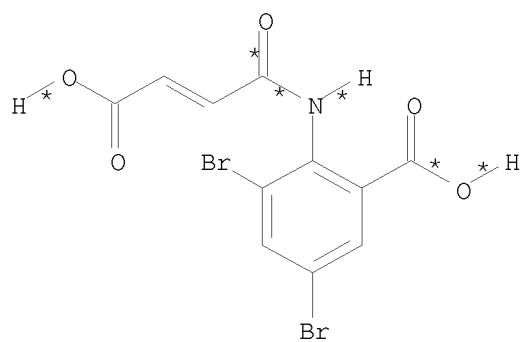
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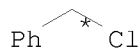
Y  
YIELD 28%

RX(2)	RCT	C 934242-55-4
	RGT	F 108-24-7 Ac2O
	PRO	E 838868-31-8
	SOL	108-24-7 Ac2O
	CON	1 hour, heated
RX(4)	RCT	E 838868-31-8
	RGT	K 5470-11-1 H2NOH-HCl
	PRO	J 934242-57-6
	SOL	110-86-1 Pyridine
	CON	3 hours, reflux
RX(10)	RCT	J 934242-57-6, X 105-39-5
	RGT	Z 584-08-7 K2CO3
	PRO	Y 934242-63-4
	SOL	67-64-1 Me2CO
	CON	24 hours, reflux

RX(83) OF 101 COMPOSED OF RX(2), RX(4), RX(11)  
RX(83) C + 2 AB ==> AC



C

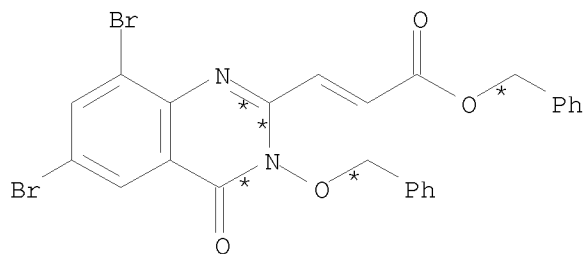


2 AB

3  
STEPS  
→



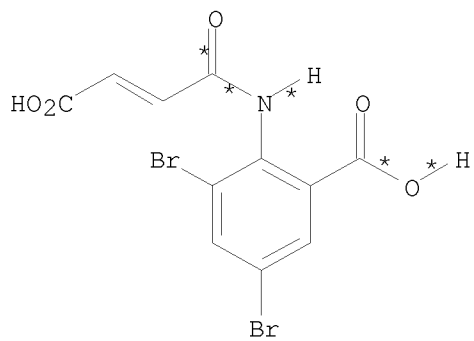
10/ 562,112



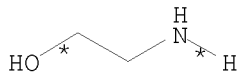
AC  
YIELD 37%

RX(2)	RCT	C 934242-55-4
	RGT	F 108-24-7 Ac2O
	PRO	E 838868-31-8
	SOL	108-24-7 Ac2O
	CON	1 hour, heated
RX(4)	RCT	E 838868-31-8
	RGT	K 5470-11-1 H2NOH-HCl
	PRO	J 934242-57-6
	SOL	110-86-1 Pyridine
	CON	3 hours, reflux
RX(11)	RCT	J 934242-57-6, AB 100-44-7
	RGT	Z 584-08-7 K2CO3
	PRO	AC 934242-64-5
	SOL	67-64-1 Me2CO
	CON	24 hours, reflux

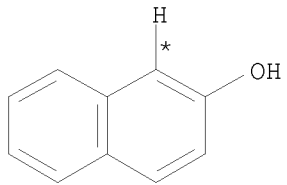
RX(84) OF 101 COMPOSED OF RX(2), RX(5), RX(12)  
RX(84) C + M + AD ==> AE



C



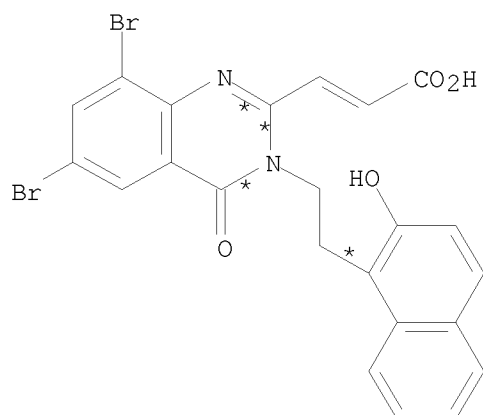
M



AD

3  
STEPS

10/ 562,112



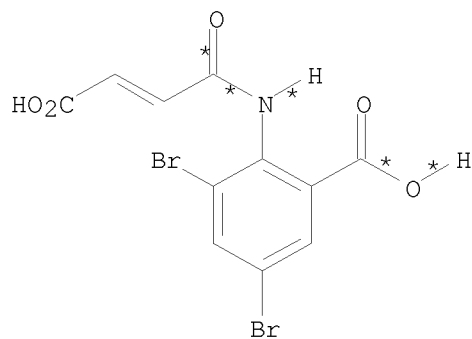
AE  
YIELD 38%

RX(2)      RCT    C 934242-55-4  
             RGT    F 108-24-7 Ac2O  
             PRO    E 838868-31-8  
             SOL    108-24-7 Ac2O  
             CON    1 hour, heated

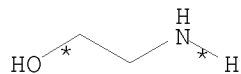
RX(5)      RCT    E 838868-31-8, M 141-43-5  
             RGT    O 127-09-3 AcONa  
             PRO    N 934242-58-7  
             SOL    64-19-7 AcOH  
             CON    3 hours, reflux

RX(12)     RCT    N 934242-58-7, AD 135-19-3  
             RGT    AF 7732-18-5 Water  
             PRO    AE 934242-65-6  
             CAT    7647-01-0 HCl  
             SOL    64-17-5 EtOH  
             CON    6 hours, heated

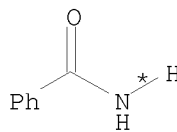
RX(85) OF 101 COMPOSED OF RX(2), RX(5), RX(13)  
RX(85)      C + M + AH ==> AI



C



M



AH

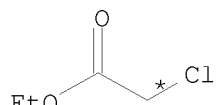
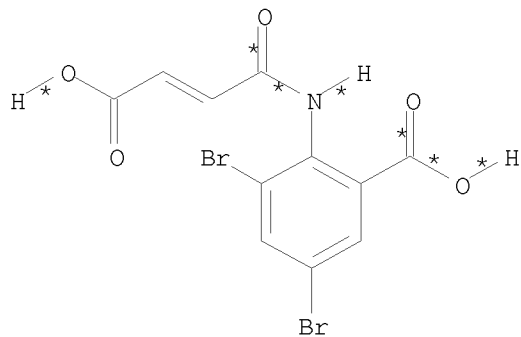


RX(2)	RCT	C 934242-55-4
	RGT	F 108-24-7 Ac2O
	PRO	E 838868-31-8
	SOL	108-24-7 Ac2O
	CON	1 hour, heated
RX(5)	RCT	E 838868-31-8, M 141-43-5
	RGT	O 127-09-3 AcONa
	PRO	N 934242-58-7
	SOL	64-19-7 AcOH
	CON	3 hours, reflux
RX(13)	RCT	N 934242-58-7, AH 55-21-0
	RGT	AF 7732-18-5 Water
	PRO	AI 934242-66-7
	CAT	7647-01-0 HCl
	SOL	64-17-5 EtOH
	CON	6 hours, heated

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RX(86) OF 101 COMPOSED OF RX(2), RX(16), RX(17)
RX(86)      C  +  2 X  ==>  AO

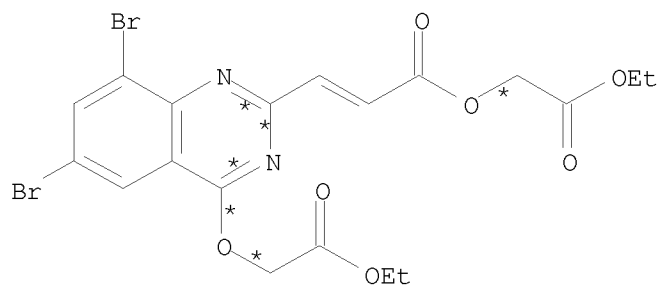
```



2 X

3  
STEPS  
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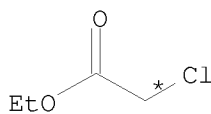
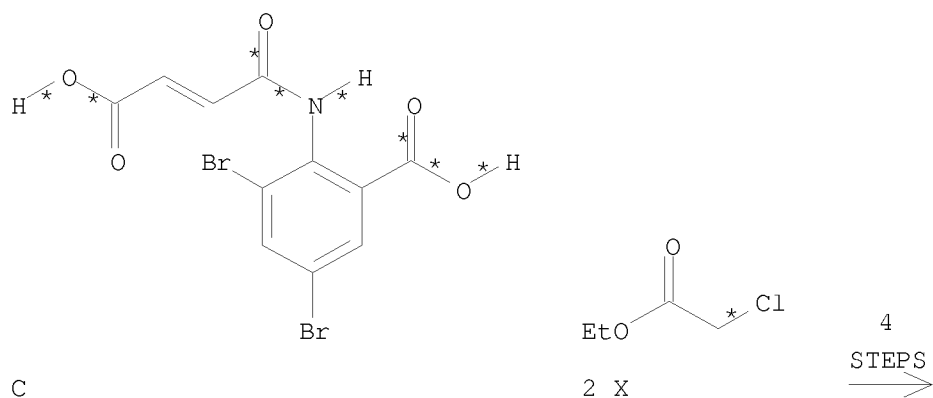
AO  
YIELD 32%

RX(2)      RCT    C 934242-55-4  
            RGT    F 108-24-7 Ac2O  
            PRO    E 838868-31-8  
            SOL    108-24-7 Ac2O  
            CON    1 hour, heated

RX(16)     RCT    E 838868-31-8  
            RGT    AN 75-12-7 Formamide  
            PRO    AM 934242-69-0  
            SOL    75-12-7 Formamide  
            CON    2 hours, reflux

RX(17)     RCT    AM 934242-69-0, X 105-39-5  
            RGT    Z 584-08-7 K2CO3  
            PRO    AO 934242-70-3  
            SOL    67-64-1 Me2CO  
            CON    25 hours, reflux

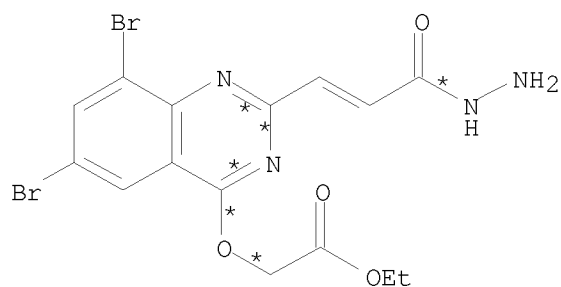
RX(100) OF 101 COMPOSED OF RX(2), RX(16), RX(17), RX(18)  
RX(100)    C    +    2 X    ==>    AP



2 X

4  
STEPS  
→

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AP  
YIELD 57%

RX(2) RCT C 934242-55-4  
RGT F 108-24-7 Ac2O  
PRO E 838868-31-8  
SOL 108-24-7 Ac2O  
CON 1 hour, heated

RX(16) RCT E 838868-31-8  
RGT AN 75-12-7 Formamide  
PRO AM 934242-69-0  
SOL 75-12-7 Formamide  
CON 2 hours, reflux

RX(17) RCT AM 934242-69-0, X 105-39-5  
RGT Z 584-08-7 K2CO3  
PRO AO 934242-70-3  
SOL 67-64-1 Me2CO  
CON 25 hours, reflux

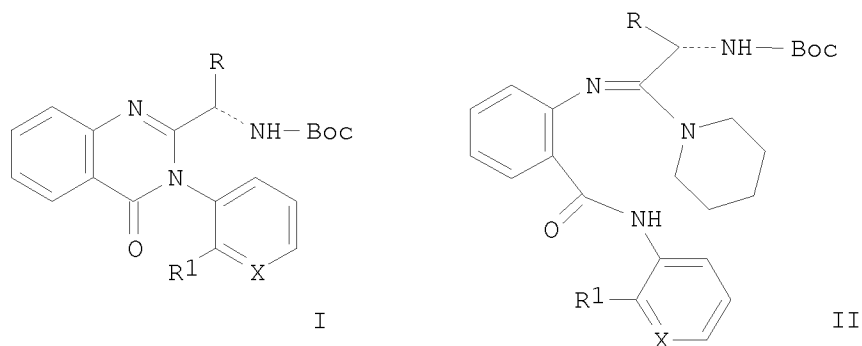
RX(18) RCT AO 934242-70-3  
RGT AQ 7803-57-8 N2H4-H2O  
PRO AP 934242-71-4  
SOL 64-17-5 EtOH  
CON 6 hours, reflux  
NTE regioselective

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 25 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 146:421939 CASREACT  
TITLE: Diastereoselective synthesis of atropisomeric 3-(2-substituted aryl)quinazolin-4-ones and their stereochemical properties  
AUTHOR(S): Tokitoh, Takashi; Kobayashi, Toshitake; Nakada, Eisuke; Inoue, Tohru; Yokoshima, Satoshi; Takahashi, Hideyo; Natsugari, Hideaki  
CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, The University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo, 113-0033, Japan  
SOURCE: Heterocycles (2006), 70, 93-99

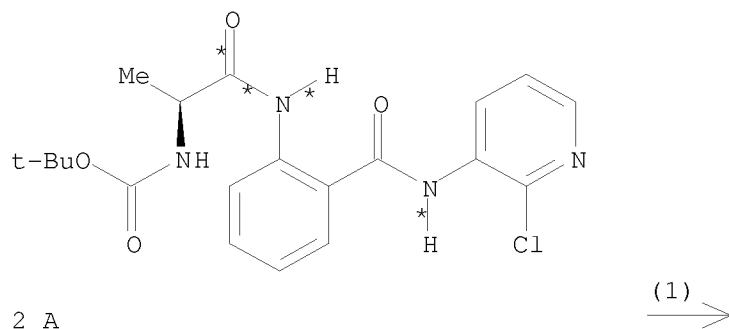
PUBLISHER:  
DOCUMENT TYPE:  
LANGUAGE:  
GI

CODEN: HTCYAM; ISSN: 0385-5414  
Japan Institute of Heterocyclic Chemistry  
Journal  
English

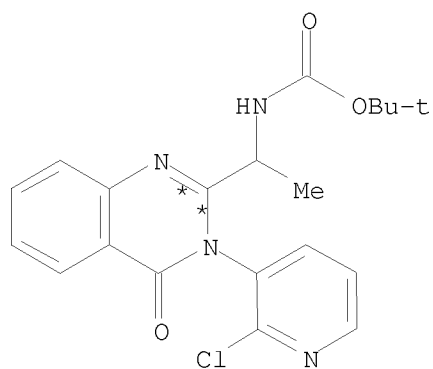


AB Atropisomeric [1-(3-aryl-4-oxo-3,4-dihydroquinazolin-2-yl)ethyl- and -phenethyl]carbamates I (X = N, R = Me, R1 = Cl; X = N, R = PhCH<sub>2</sub>, R1 = Cl; X = CH, R = PhCH<sub>2</sub>, R1 = CO<sub>2</sub>Me) were diastereoselectively synthesized by acid-catalyzed cyclization of appropriate {2-[(arylcarbamoyl)phenylimino]-1-methyl- and -1-benzyl-2-piperidin-1-yl}carbamates II. Investigation of the stereochem. properties of I revealed that both atropisomers have high stereochem. stability and the (aR\*, S\*)- is stereochem. more stable than the isomeric (aS\*, S\*)-form.

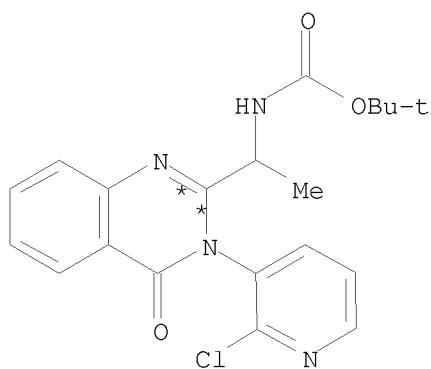
RX(1) OF 30 ...2 A ==> B + C



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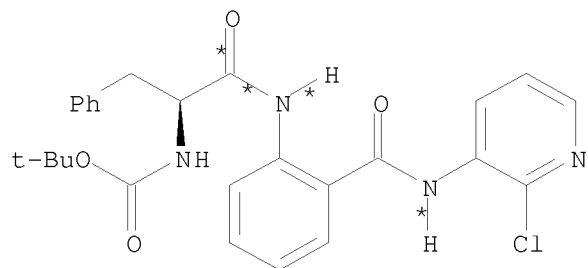
B  
YIELD 38%



C  
YIELD 42%

RX(1)      RCT    A 934167-98-3  
             RGT    D 121-44-8 Et3N, E 75-77-4 Me3SiCl  
             PRO    B 934170-26-0, C 934170-27-1  
             SOL    107-06-2 ClCH2CH2Cl  
             CON    28 hours, 80 deg C

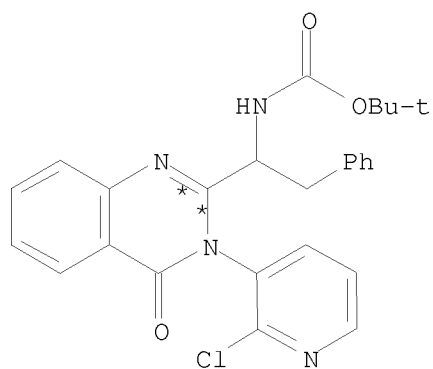
RX(3) OF 30      ...M ==> N



M

(3)  $\longrightarrow$

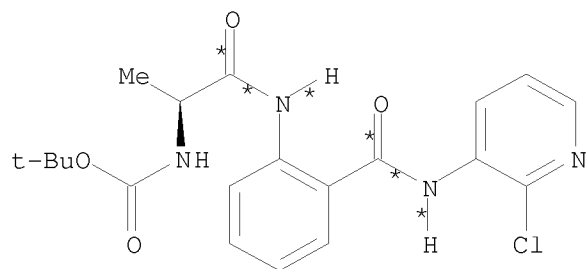
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N  
YIELD 70%

RX(3) RCT M 934167-99-4  
RGT D 121-44-8 Et3N, E 75-77-4 Me3SiCl  
PRO N 934170-28-2  
SOL 107-06-2 ClCH2CH2Cl  
CON 28 hours, 80 deg C

RX(19) OF 30 COMPOSED OF RX(9), RX(2)  
RX(19) 2 A ==> B + C

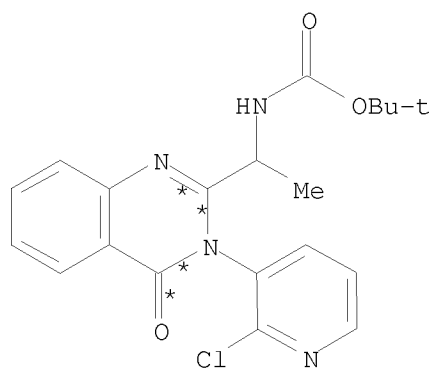


2 A

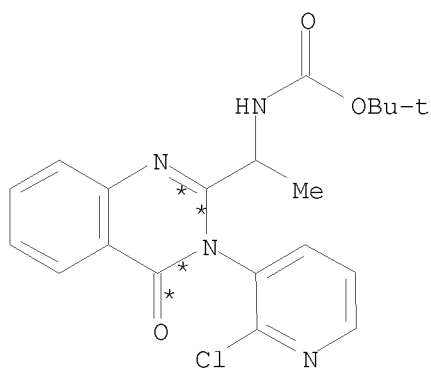
2  
STEPS  
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B  
YIELD 58%



C  
YIELD 14%

RX(9) RCT A 934167-98-3  
RGT Y 7087-68-5 EtN(Pr-i)2, Z 7553-56-2 I2, AA 603-35-0 PPh3  
PRO G 941569-73-9  
SOL 75-09-2 CH2Cl2  
CON 0.5 hours, room temperature

RX(2) RCT G 941569-73-9

STAGE(1)

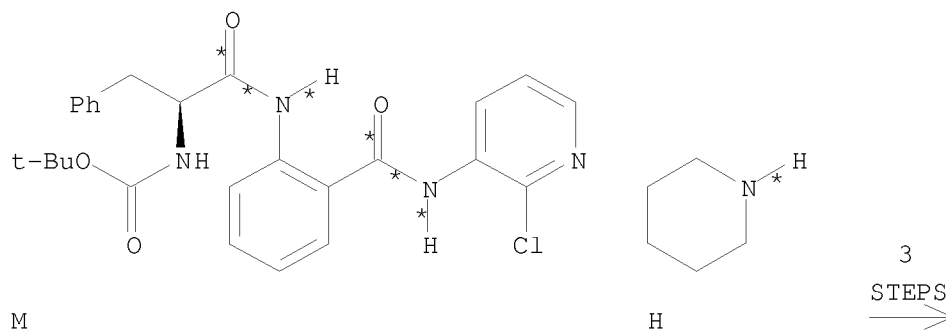
RGT H 110-89-4 Piperidine  
SOL 141-78-6 AcOEt  
CON 15 hours, room temperature

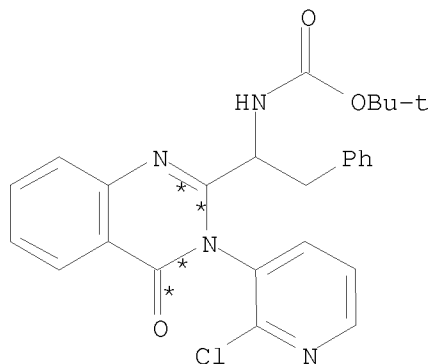
STAGE(2)

RGT I 7646-93-7 KHSO4  
SOL 7732-18-5 Water, 123-91-1 Dioxane  
CON overnight, room temperature

PRO B 934170-26-0, C 934170-27-1  
NTE stereoselective

RX(28) OF 30 COMPOSED OF RX(10), RX(13), RX(4)  
RX(28) M + H ==> N





N  
YIELD 100%

RX(10) RCT M 934167-99-4  
RGT Y 7087-68-5 EtN(Pr-i)2, Z 7553-56-2 I2, AA 603-35-0 PPh3  
PRO AB 941570-09-8  
SOL 75-09-2 CH2Cl2  
CON 0.5 hours, room temperature

RX(13) RCT AB 941570-09-8, H 110-89-4  
PRO O 934168-01-1  
SOL 141-78-6 AcOEt  
CON 15 hours, room temperature

RX(4) RCT O 934168-01-1  
RGT P 7631-86-9 SiO2  
PRO N 934170-28-2  
SOL 67-66-3 CHCl3  
CON 5 days, room temperature  
NTE stereoselective, silica gel used

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 26 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 146:421925 CASREACT

TITLE: Synthesis and antimicrobial activity of some sulfonamides and aryl amides

AUTHOR(S): Radadia, V. R.; Purohit, D. M.; Patolia, V. N.

CORPORATE SOURCE: Chemistry Department, Kamani Science College, Amreli, 365 601, India

SOURCE: Journal of the Institution of Chemists (India) (2006), 78(1), 8-11

CODEN: JOICA7; ISSN: 0020-3254

PUBLISHER: Institution of Chemists (India)

DOCUMENT TYPE: Journal

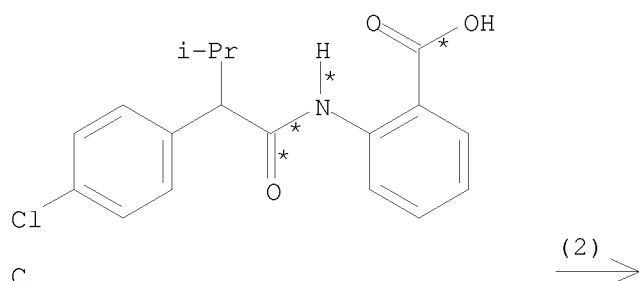
LANGUAGE: English

AB Some new N-4-oxoquinazolin-3-yl sulfonamides and aryl amides were prepared and the constitution of the products were supported by IR, NMR, and mass

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spectra. The products were screened for their antimicrobial activity compared with standard drugs. All the compds. showed moderate activity.

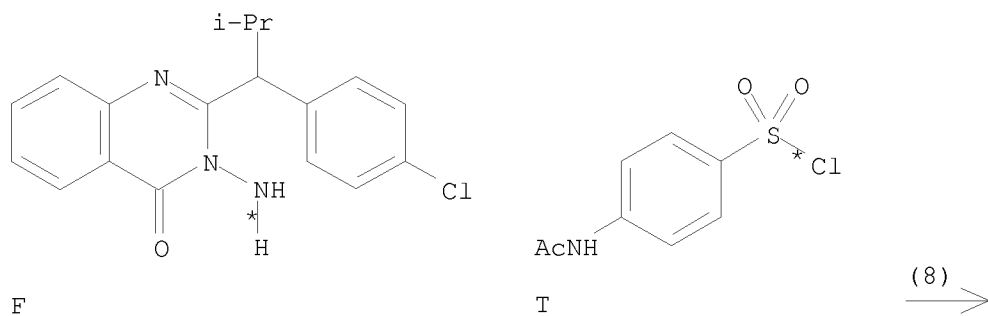
RX(2) OF 60 ...C ==> F...



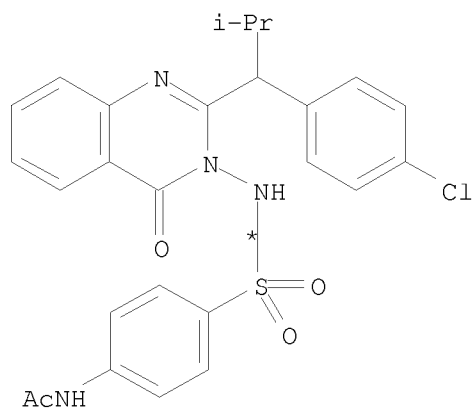
F  
YIELD 86%

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(8) OF 60 ...F + T ==> U



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U  
YIELD 90%

RX(8) RCT F 934216-72-5, T 121-60-8

STAGE(1)

RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

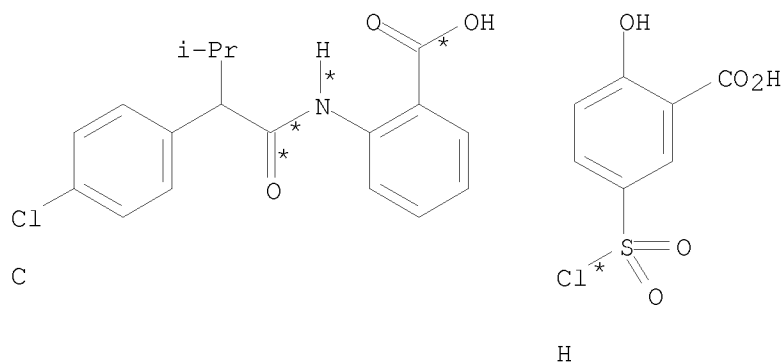
STAGE(2)

RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

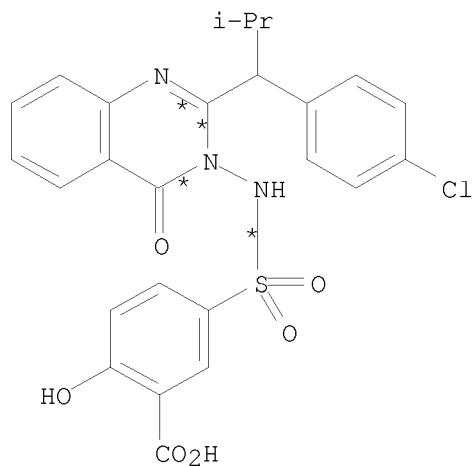
PRO U 934216-78-1

RX(23) OF 60 COMPOSED OF RX(2), RX(3)

RX(23) C + H ==> I



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I  
YIELD 90%

RX(2)      RCT    C 851191-19-0  
            RGT    G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
            PRO    F 934216-72-5  
            SOL    64-17-5 EtOH  
            CON    4 hours, reflux

RX(3)      RCT    F 934216-72-5, H 17243-13-9

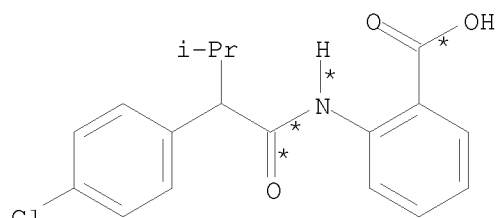
STAGE(1)  
            RGT    D 110-86-1 Pyridine  
            SOL    110-86-1 Pyridine  
            CON    5 hours, reflux

STAGE(2)  
            RGT    J 7647-01-0 HCl  
            SOL    7732-18-5 Water  
            CON    room temperature, neutralized

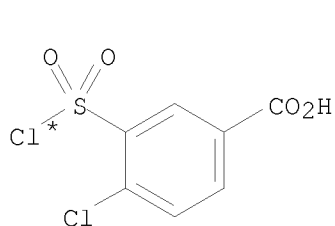
PRO    I 934216-73-6

RX(24) OF 60 COMPOSED OF RX(2), RX(4)

RX(24)      C    +    L    ==>    M



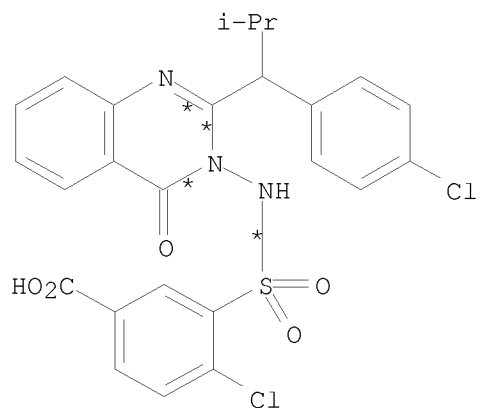
C



L

2  
STEPS  
→

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M  
YIELD 90%

RX(2)      RCT    C 851191-19-0  
             RGT    G 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O, D 110-86-1 Pyridine  
             PRO    F 934216-72-5  
             SOL    64-17-5 EtOH  
             CON    4 hours, reflux

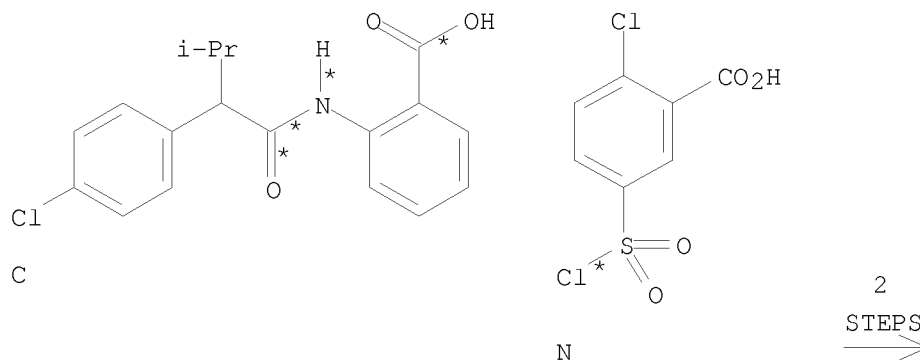
RX(4)      RCT    F 934216-72-5, L 2494-79-3

STAGE(1)  
             RGT    D 110-86-1 Pyridine  
             SOL    110-86-1 Pyridine  
             CON    5 hours, reflux

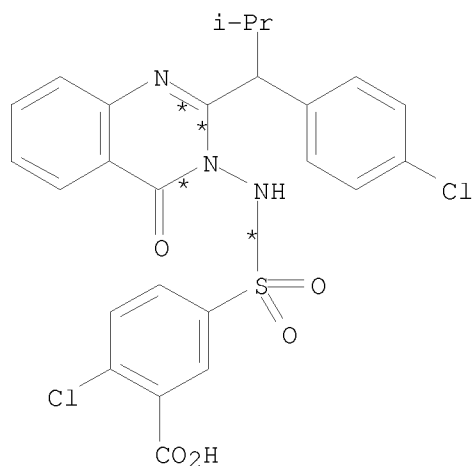
STAGE(2)  
             RGT    J 7647-01-0 HCl  
             SOL    7732-18-5 Water  
             CON    room temperature, neutralized

PRO    M 934216-74-7

RX(25) OF 60 COMPOSED OF RX(2), RX(5)  
RX(25)      C    +    N    ==>    O



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O  
YIELD 90%

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

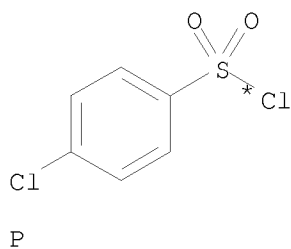
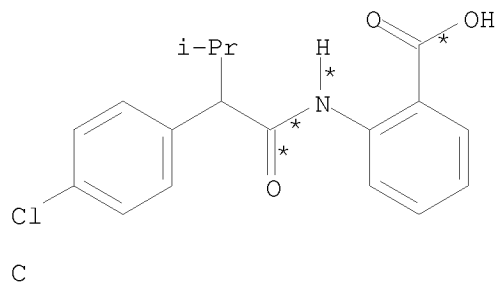
RX(5) RCT F 934216-72-5, N 137-64-4

STAGE(1)  
RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

STAGE(2)  
RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

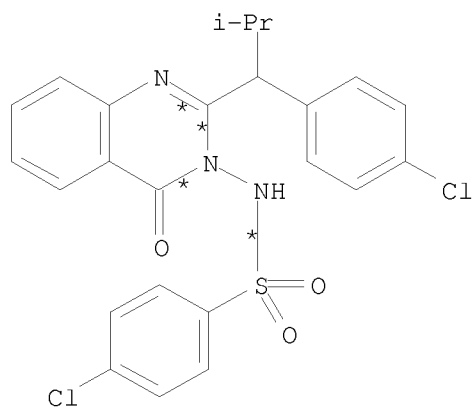
PRO O 934216-75-8

RX(26) OF 60 COMPOSED OF RX(2), RX(6)  
RX(26) C + P ==> Q



2  
STEPS  
→

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Q  
YIELD 90%

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

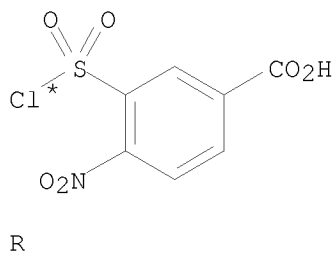
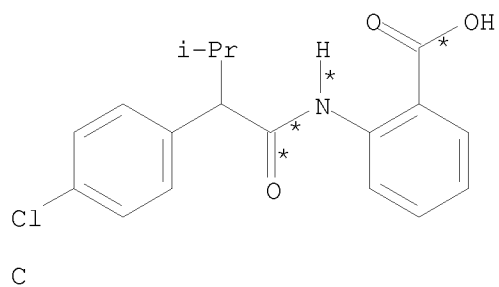
RX(6) RCT F 934216-72-5, P 98-60-2

STAGE(1)  
RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

STAGE(2)  
RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

PRO Q 934216-76-9

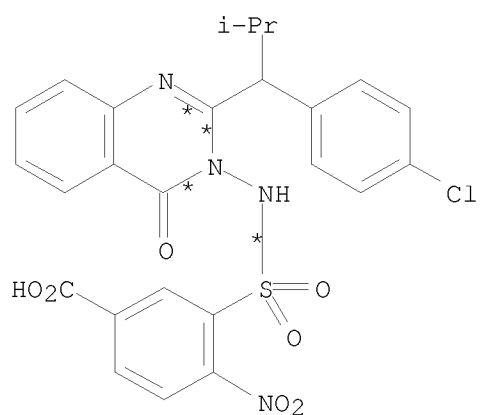
RX(27) OF 60 COMPOSED OF RX(2), RX(7)  
RX(27) C + R ==> S



2  
STEPS  
→



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S  
YIELD 79%

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(7) RCT F 934216-72-5, R 871243-31-1

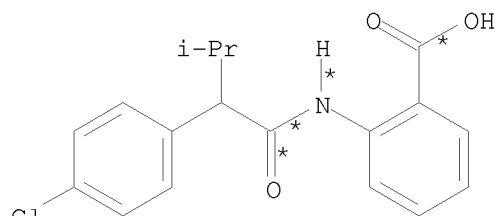
STAGE(1)  
RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

STAGE(2)  
RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

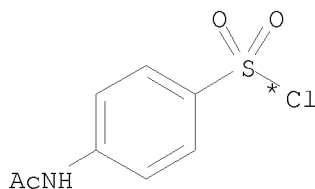
PRO S 934216-77-0

RX(28) OF 60 COMPOSED OF RX(2), RX(8)

RX(28) C + T ==> U



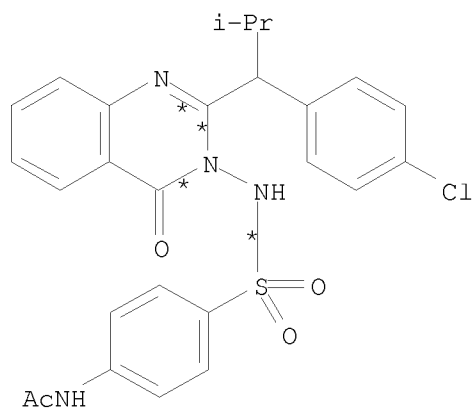
C



T

2  
STEPS  
→

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U  
YIELD 90%

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(8) RCT F 934216-72-5, T 121-60-8

STAGE(1)

RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

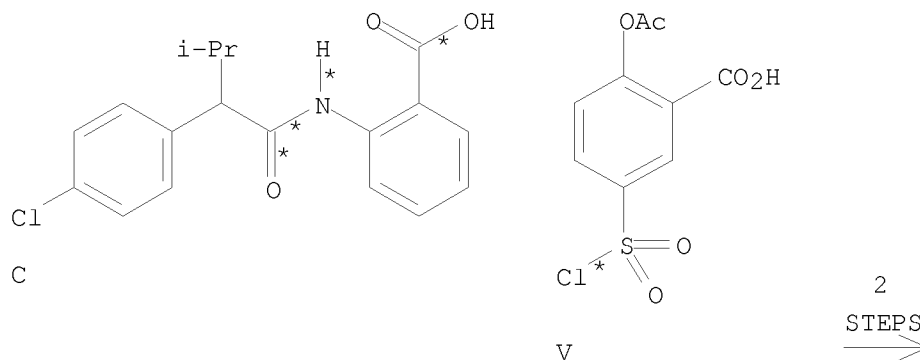
STAGE(2)

RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

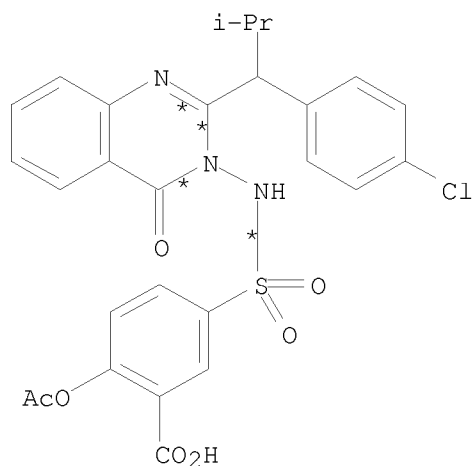
PRO U 934216-78-1

RX(29) OF 60 COMPOSED OF RX(2), RX(9)

RX(29) C + V ==> W



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W  
YIELD 90%

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

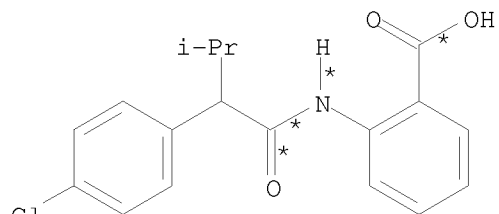
RX(9) RCT F 934216-72-5, V 77718-41-3

STAGE(1)  
RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

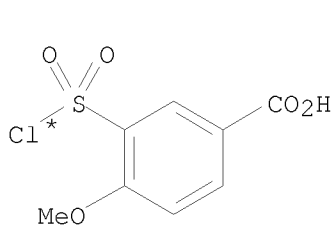
STAGE(2)  
RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

PRO W 934216-79-2

RX(30) OF 60 COMPOSED OF RX(2), RX(10)  
RX(30) C + X ==> Y



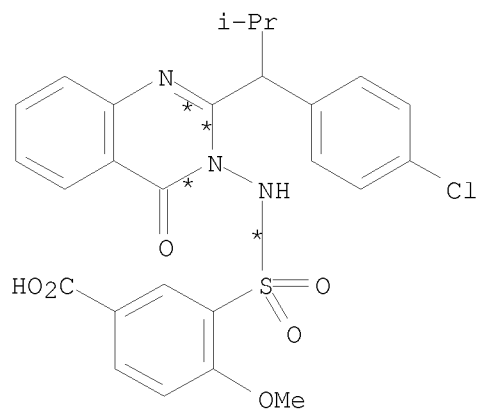
C



X

2  
STEPS  
→

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Y  
YIELD 90%

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(10) RCT F 934216-72-5, X 50803-29-7

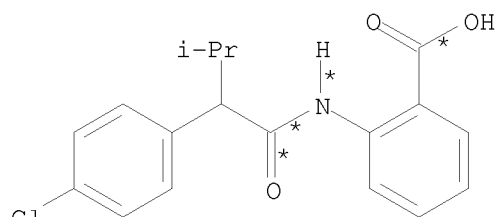
STAGE(1)  
RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

STAGE(2)  
RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

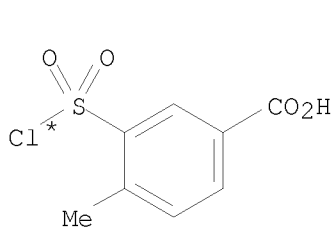
PRO Y 934216-80-5

RX(31) OF 60 COMPOSED OF RX(2), RX(11)

RX(31) C + Z ==> AA



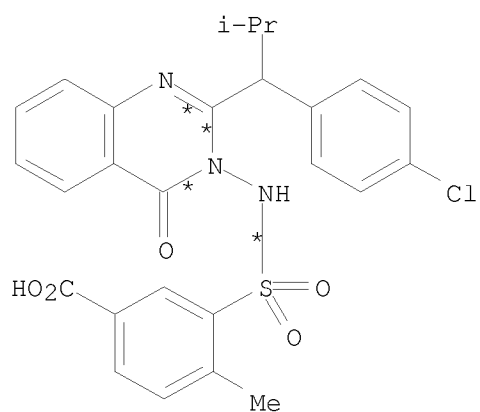
C



Z

2  
STEPS  
→

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AA  
YIELD 90%

RX(2)      RCT    C 851191-19-0  
            RGT    G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
            PRO    F 934216-72-5  
            SOL    64-17-5 EtOH  
            CON    4 hours, reflux

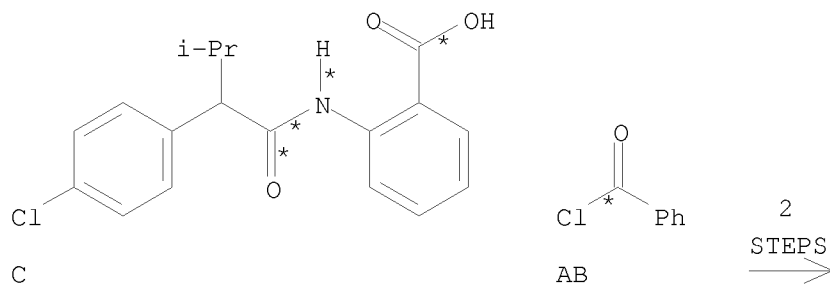
RX(11)      RCT    F 934216-72-5, Z 2548-29-0

STAGE(1)  
            RGT    D 110-86-1 Pyridine  
            SOL    110-86-1 Pyridine  
            CON    5 hours, reflux

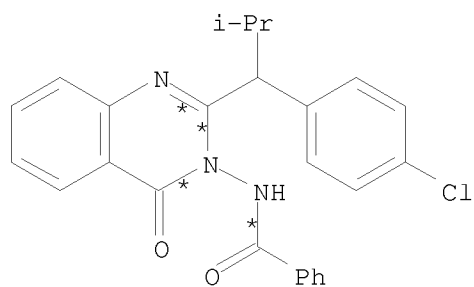
STAGE(2)  
            RGT    J 7647-01-0 HCl  
            SOL    7732-18-5 Water  
            CON    room temperature, neutralized

PRO    AA 934216-81-6

RX(32) OF 60 COMPOSED OF RX(2), RX(12)  
RX(32)      C    +    AB    ==>    AC



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AC  
YIELD 75%

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(12) RCT F 934216-72-5, AB 98-88-4

STAGE(1)

RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

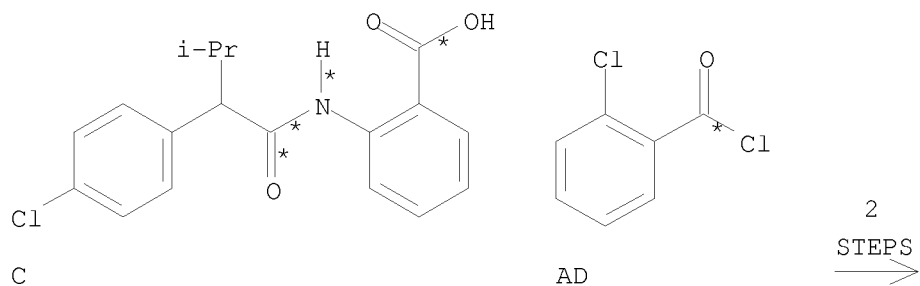
STAGE(2)

RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

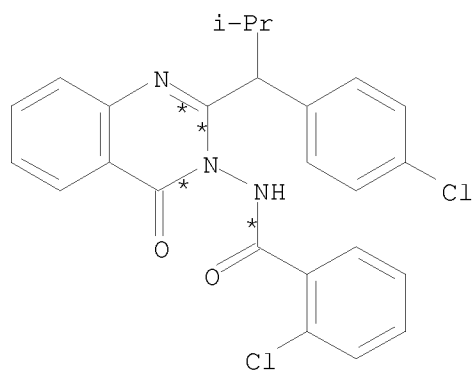
PRO AC 934216-82-7

RX(33) OF 60 COMPOSED OF RX(2), RX(13)

RX(33) C + AD ==> AE



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AE  
YIELD 75%

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(13) RCT F 934216-72-5, AD 609-65-4

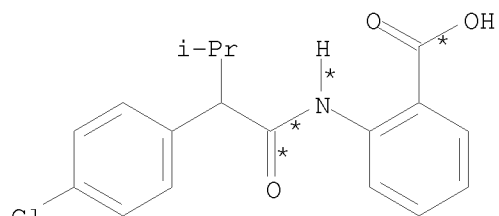
STAGE(1)  
RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

STAGE(2)  
RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

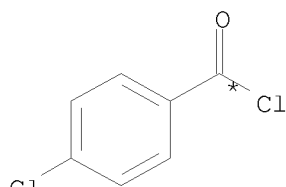
PRO AE 934216-83-8

RX(34) OF 60 COMPOSED OF RX(2), RX(14)

RX(34) C + AF ==> AG



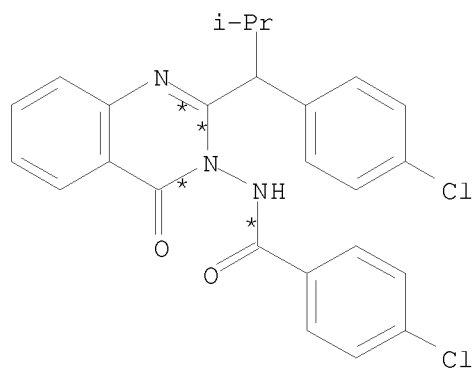
C



AF

2  
STEPS  
→

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AG  
YIELD 75%

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(14) RCT F 934216-72-5, AF 122-01-0

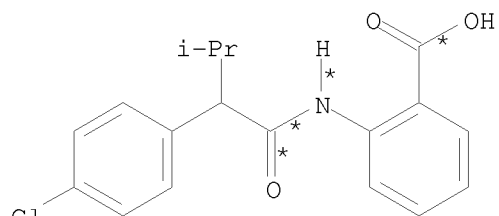
STAGE(1)  
RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

STAGE(2)  
RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

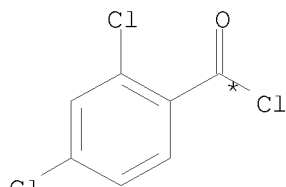
PRO AG 934216-84-9

RX(35) OF 60 COMPOSED OF RX(2), RX(15)

RX(35) C + AH ==> AI



C

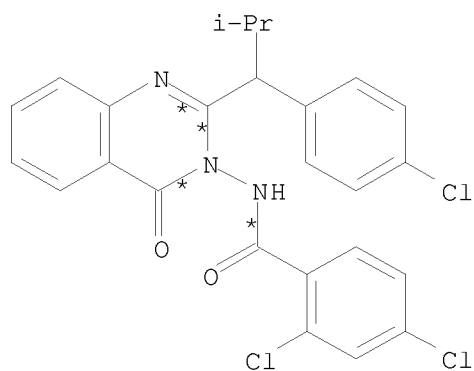


AH

2  
STEPS  
→



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AI  
YIELD 75%

RX(2)      RCT    C 851191-19-0  
            RGT    G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
            PRO    F 934216-72-5  
            SOL    64-17-5 EtOH  
            CON    4 hours, reflux

RX(15)     RCT    F 934216-72-5, AH 89-75-8

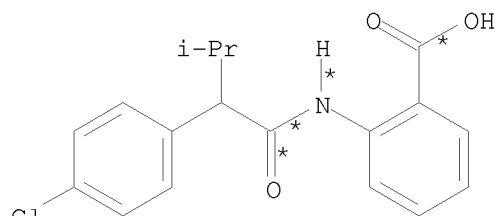
STAGE(1)  
            RGT    D 110-86-1 Pyridine  
            SOL    110-86-1 Pyridine  
            CON    5 hours, reflux

STAGE(2)  
            RGT    J 7647-01-0 HCl  
            SOL    7732-18-5 Water  
            CON    room temperature, neutralized

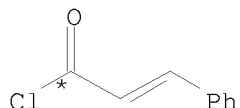
PRO    AI 934216-85-0

RX(36) OF 60 COMPOSED OF RX(2), RX(16)

RX(36)      C    +    AJ    ==>    AK



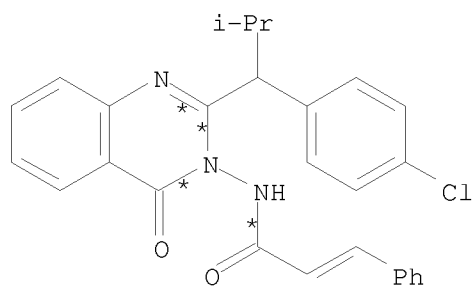
C



AJ

2  
STEPS  
→

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AK  
YIELD 75%

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(16) RCT F 934216-72-5, AJ 102-92-1

STAGE(1)

RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

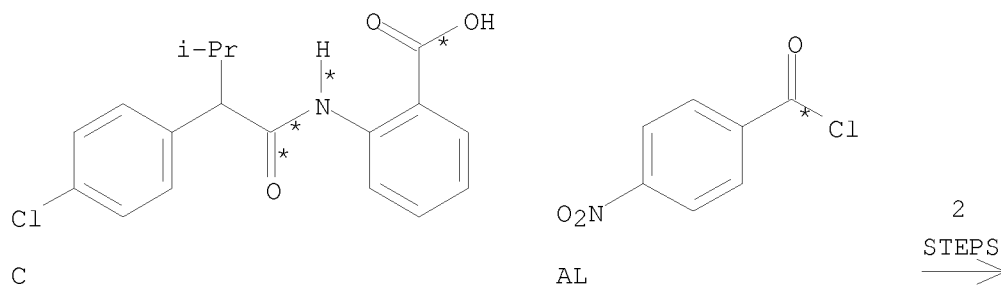
STAGE(2)

RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

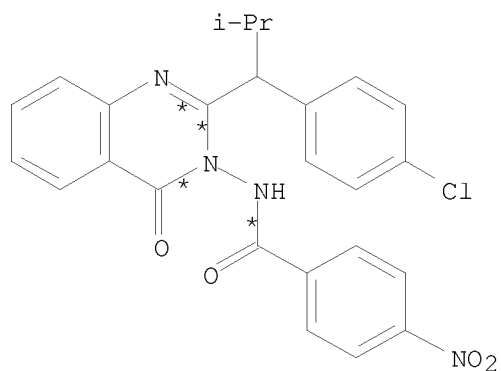
PRO AK 934216-86-1

RX(37) OF 60 COMPOSED OF RX(2), RX(17)

RX(37) C + AL ==> AM



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AM  
YIELD 69%

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(17) RCT F 934216-72-5, AL 122-04-3

STAGE(1)

RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

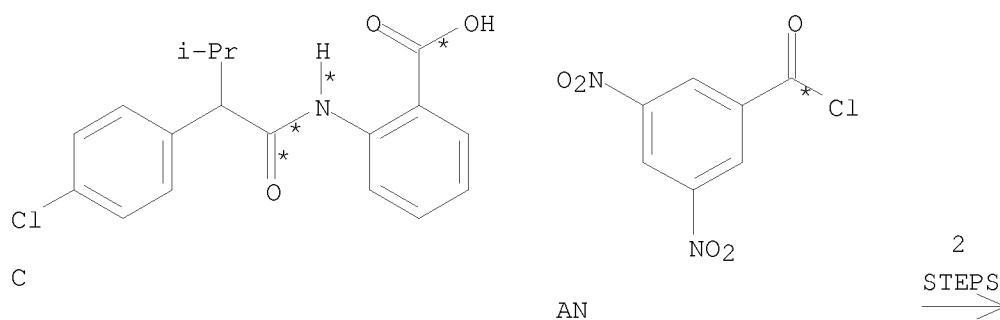
STAGE(2)

RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

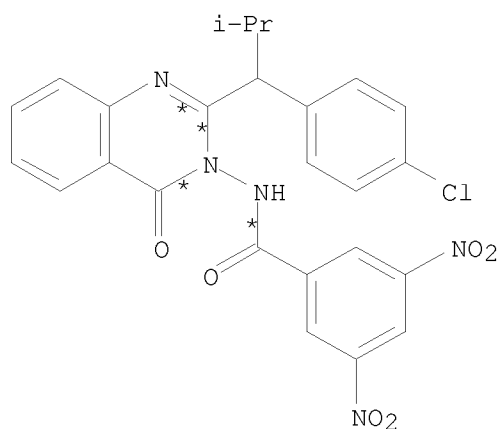
PRO AM 934216-87-2

RX(38) OF 60 COMPOSED OF RX(2), RX(18)

RX(38) C + AN ==> AO



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AO  
YIELD 75%

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

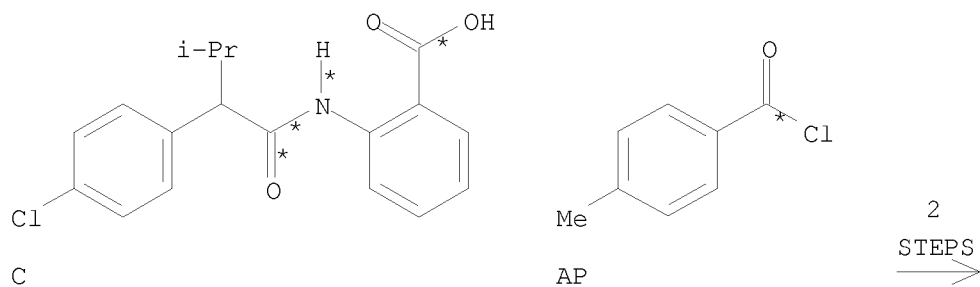
RX(18) RCT F 934216-72-5, AN 99-33-2

STAGE(1)  
RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

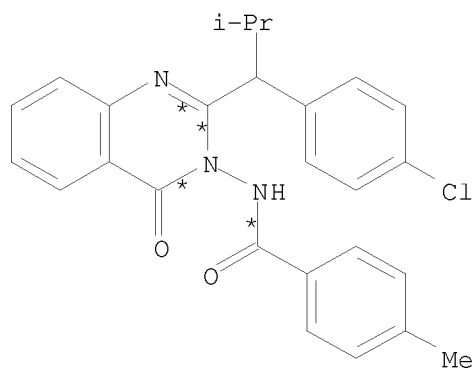
STAGE(2)  
RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

PRO AO 934216-88-3

RX(39) OF 60 COMPOSED OF RX(2), RX(19)  
RX(39) C + AP ==> AQ



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AQ  
YIELD 75%

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(19) RCT F 934216-72-5, AP 874-60-2

STAGE(1)

RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

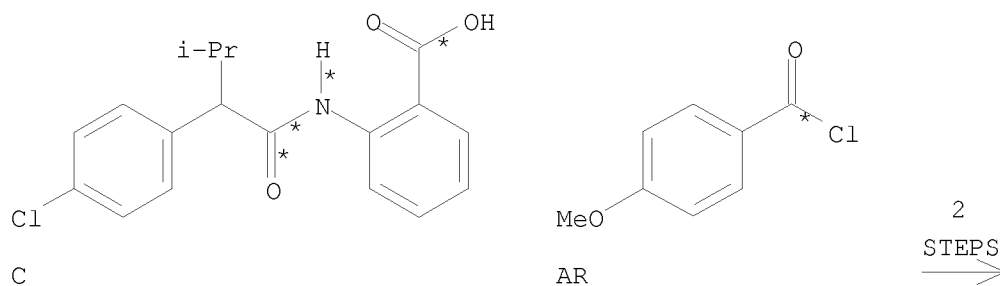
STAGE(2)

RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

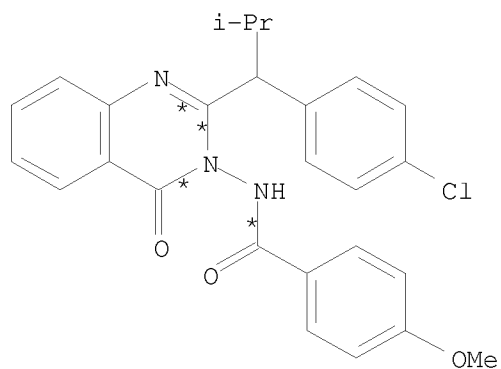
PRO AQ 934216-89-4

RX(40) OF 60 COMPOSED OF RX(2), RX(20)

RX(40) C + AR ==> AS



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AS  
YIELD 75%

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(20) RCT F 934216-72-5, AR 100-07-2

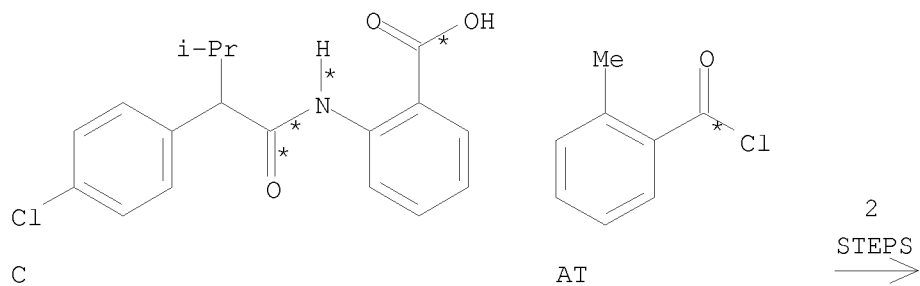
STAGE(1)  
RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

STAGE(2)  
RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

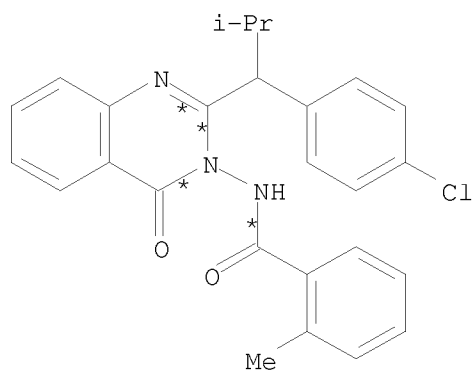
PRO AS 934216-90-7

RX(41) OF 60 COMPOSED OF RX(2), RX(21)

RX(41) C + AT ==> AU



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AU  
YIELD 75%

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(21) RCT F 934216-72-5, AT 933-88-0

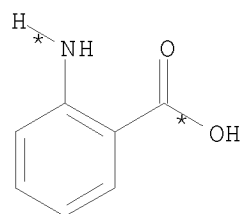
STAGE(1)  
RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

STAGE(2)  
RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

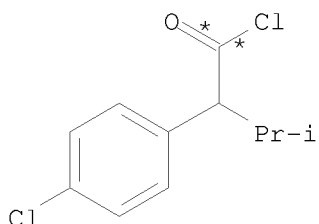
PRO AU 934216-91-8

RX(47) OF 60 COMPOSED OF RX(1), RX(2), RX(8)

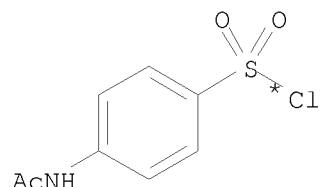
RX(47) A + B + T ==> U



A



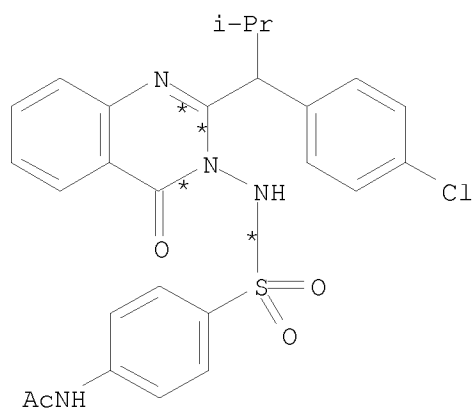
B



T

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3  
STEPS  
→



U  
YIELD 90%

RX(1) RCT A 118-92-3, B 51631-50-6  
RGT D 110-86-1 Pyridine  
PRO C 851191-19-0  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(2) RCT C 851191-19-0  
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine  
PRO F 934216-72-5  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(8) RCT F 934216-72-5, T 121-60-8

STAGE(1)

RGT D 110-86-1 Pyridine  
SOL 110-86-1 Pyridine  
CON 5 hours, reflux

STAGE(2)

RGT J 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, neutralized

PRO U 934216-78-1

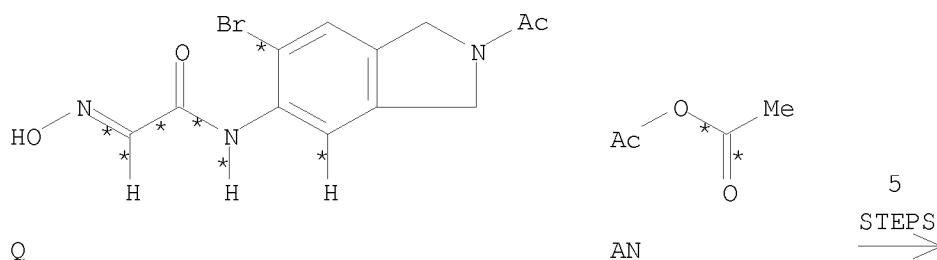
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



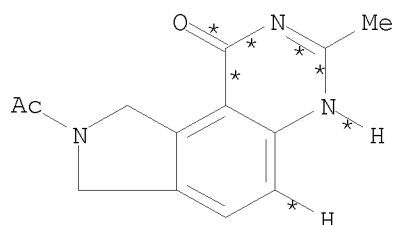
ACCESSION NUMBER: 146:414392 CASREACT  
 TITLE: Synthesis of dihydropyrrolo[3,4-f]quinazoline  
 antifolates and their antitumor activity in vitro  
 AUTHOR(S): Baek, Du-Jong  
 CORPORATE SOURCE: Department of Chemistry, College of Natural Sciences,  
 Sangmyung University, 7 Hongji-Dong, Chongro-Gu,  
 Seoul, 110-743, S. Korea  
 SOURCE: Yakhak Hoechi (2006), 50(4), 278-286  
 CODEN: YAHOA3; ISSN: 0377-9556  
 PUBLISHER: Pharmaceutical Society of Korea  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Korean

AB Classical dihydropyrrolo[3,4-f]quinazoline antifolates 7, 8 and 9, in which the tricyclic ring is structurally similar to the pteridine ring of CH<sub>2</sub>-THF (1), the cofactor of thymidylate synthase (TS), were synthesized, and their in vitro antitumor activity was evaluated by measuring the cell growth inhibitory activity against cancer cell lines. The target compds. were cytotoxic against CCRF-CEM, human T-cell acute lymphoblastic leukemia, with the cell growth inhibitory activity (IC<sub>50</sub>) of 0.8 .apprx. 8.3  $\mu$ M. Among the three compds., 3-amino analog 7 was 10- and 3.5-fold more cytotoxic compared to the 3-Me analogs 8 and 9, and its cytotoxicity was similar to that of the reference compound with the IC<sub>50</sub> value of 0.83  $\mu$ M. This result was supposed as the consequence of the fact that dihydropyrroloquinazolinone ring with amino group was able to bind well in the active site of TS. In the case of 3-Me analogs, analog 9, which has two-carbon bridge between the dihydropyrroloquinazolinone ring and benzoyl-L-glutamic acid, was 3-times more potent in cytotoxicity than analog 8 which has one-carbon bridge, and this result indicates that the distance and conformational orientation of the benzoyl-L-glutamic acid moiety with respect to the tricyclic ring may also be a crucial determinant of cell growth inhibitory activity.

RX(108) OF 219 COMPOSED OF RX(6), RX(7), RX(8), RX(15), RX(16)  
 RX(108) Q + AN ==> AP



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AP  
YIELD 84%

RX(6) RCT Q 934186-17-1  
RGT H 7664-93-9 H2SO4  
PRO V 934186-18-2  
SOL 7732-18-5 Water  
CON 2 hours, 80 deg C

RX(7) RCT V 934186-18-2  
RGT X 1310-73-2 NaOH, Y 7722-84-1 H2O2  
PRO W 934186-19-3  
SOL 7732-18-5 Water  
CON 1 hour, 80 deg C

RX(8) RCT W 934186-19-3  
RGT J 1333-74-0 H2  
PRO Z 934186-20-6  
CAT 7440-05-3 Pd  
SOL 67-56-1 MeOH, 109-99-9 THF  
CON 2 hours, room temperature

RX(15) RCT Z 934186-20-6, AN 108-24-7  
PRO AO 934186-27-3  
CON 4 hours, 110 deg C

RX(16) RCT AO 934186-27-3

STAGE(1)

RGT AQ 7664-41-7 NH3  
CON 3 hours, -78 deg C

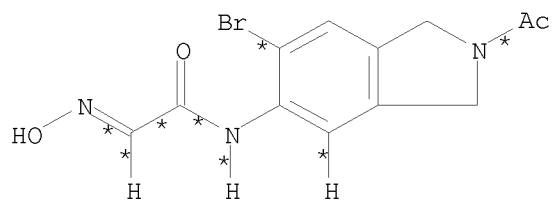
STAGE(2)

RGT X 1310-73-2 NaOH  
SOL 7732-18-5 Water  
CON 1 hour, reflux

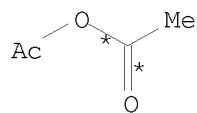
PRO AP 934186-28-4

RX(109) OF 219 COMPOSED OF RX(6), RX(7), RX(8), RX(15), RX(18)  
RX(109) Q + AN + AK ==> AS

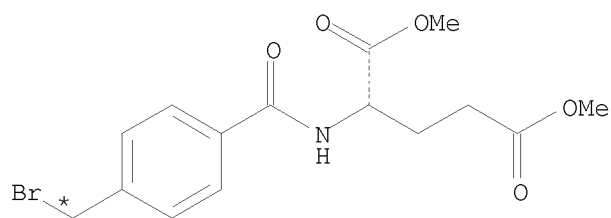
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Q

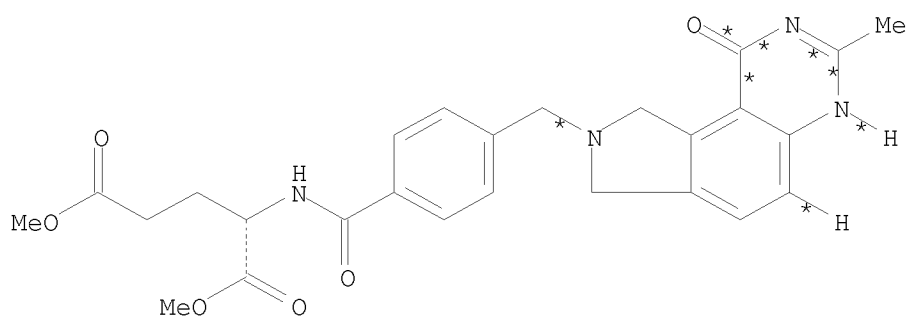


AN



AK

5  
STEPS  
→



AS  
YIELD 48%

RX(6)      RCT    Q 934186-17-1  
              RGT    H 7664-93-9 H2SO4  
              PRO    V 934186-18-2  
              SOL    7732-18-5 Water  
              CON    2 hours, 80 deg C

RX(7)      RCT    V 934186-18-2  
              RGT    X 1310-73-2 NaOH, Y 7722-84-1 H2O2  
              PRO    W 934186-19-3  
              SOL    7732-18-5 Water  
              CON    1 hour, 80 deg C

RX(8)      RCT    W 934186-19-3  
              RGT    J 1333-74-0 H2  
              PRO    Z 934186-20-6  
              CAT    7440-05-3 Pd

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SOL 67-56-1 MeOH, 109-99-9 THF  
CON 2 hours, room temperature

RX(15) RCT Z 934186-20-6, AN 108-24-7  
PRO AO 934186-27-3  
CON 4 hours, 110 deg C

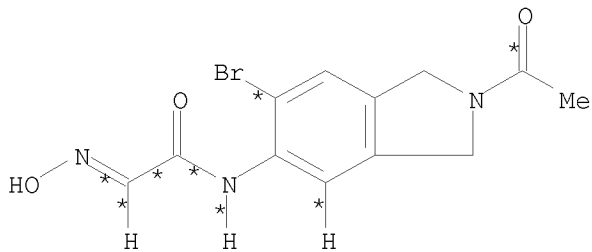
RX(18) RCT AO 934186-27-3

STAGE(1)  
RGT D 121-44-8 Et3N  
SOL 68-12-2 DMF  
CON 30 minutes, room temperature

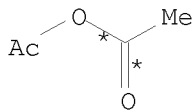
STAGE(2)  
RCT AK 934186-24-0  
CON 12 hours, room temperature

PRO AS 934186-30-8

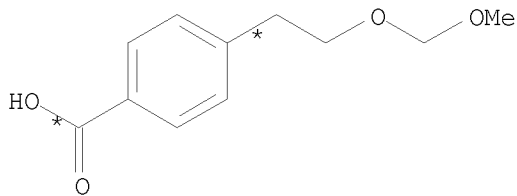
RX(110) OF 219 COMPOSED OF RX(6), RX(7), RX(8), RX(15), RX(21)

$$RX(110) \quad Q + AN + AY + AZ \implies BA$$


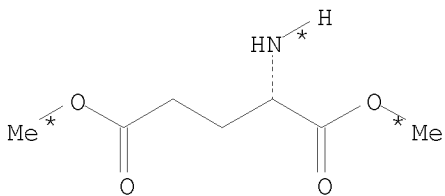
Q



AN



AY

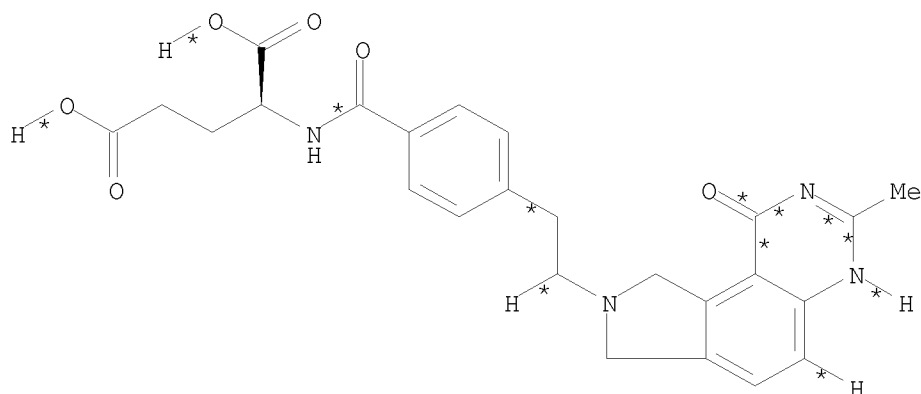


AZ

5

STEPS

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BA  
YIELD 81%

RX(6) RCT Q 934186-17-1  
RGT H 7664-93-9 H2SO4  
PRO V 934186-18-2  
SOL 7732-18-5 Water  
CON 2 hours, 80 deg C

RX(7) RCT V 934186-18-2  
RGT X 1310-73-2 NaOH, Y 7722-84-1 H2O2  
PRO W 934186-19-3  
SOL 7732-18-5 Water  
CON 1 hour, 80 deg C

RX(8) RCT W 934186-19-3  
RGT J 1333-74-0 H2  
PRO Z 934186-20-6  
CAT 7440-05-3 Pd  
SOL 67-56-1 MeOH, 109-99-9 THF  
CON 2 hours, room temperature

RX(15) RCT Z 934186-20-6, AN 108-24-7  
PRO AO 934186-27-3  
CON 4 hours, 110 deg C

RX(21) RCT AO 934186-27-3, AY 934186-33-1

STAGE(1)  
RGT D 121-44-8 Et3N, BB 75-75-2 MeSO3H  
SOL 75-09-2 CH2Cl2  
CON SUBSTAGE(1) 0 - 5 deg C  
SUBSTAGE(2) 10 minutes, 0 - 5 deg C

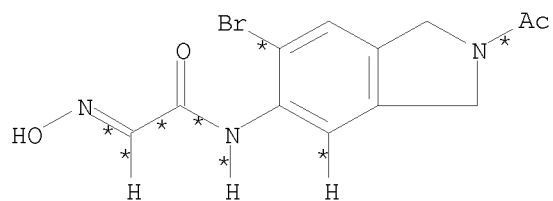
STAGE(2)  
RCT AZ 6525-53-7  
CON 1 hour

PRO BA 934186-31-9

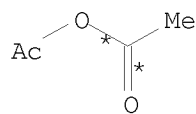
RX(111) OF 219 COMPOSED OF RX(6), RX(7), RX(8), RX(15), RX(22)

10/ 562,112

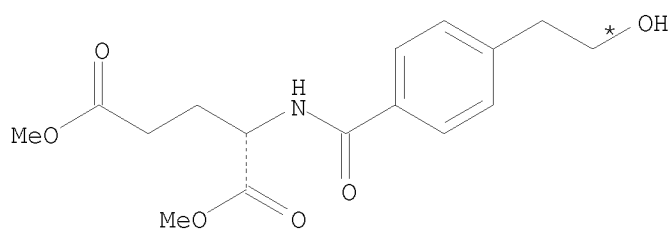
RX(111) Q + AN + BC ==> BD



Q

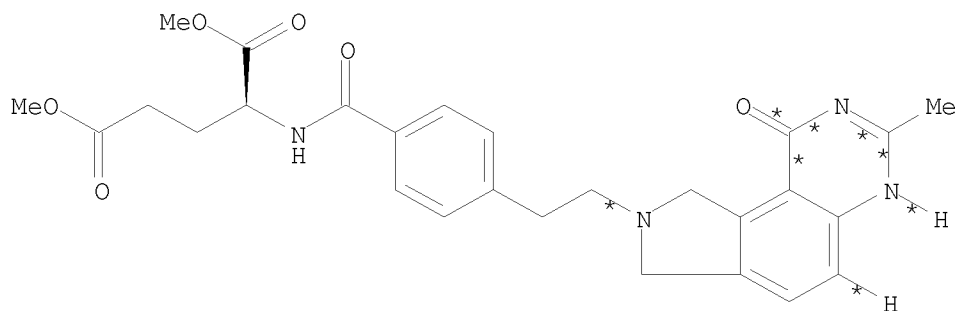


AN



BC

5  
STEPS  
→



BD

YIELD 33%

RX(6) RCT Q 934186-17-1  
RGT H 7664-93-9 H2SO4  
PRO V 934186-18-2  
SOL 7732-18-5 Water  
CON 2 hours, 80 deg C

RX(7) RCT V 934186-18-2  
RGT X 1310-73-2 NaOH, Y 7722-84-1 H2O2  
PRO W 934186-19-3  
SOL 7732-18-5 Water  
CON 1 hour, 80 deg C

RX(8) RCT W 934186-19-3  
RGT J 1333-74-0 H2

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PRO Z 934186-20-6  
CAT 7440-05-3 Pd  
SOL 67-56-1 MeOH, 109-99-9 THF  
CON 2 hours, room temperature

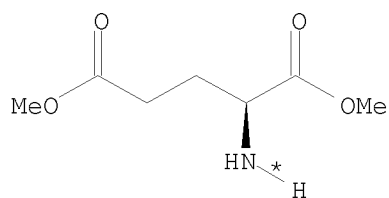
RX(15) RCT Z 934186-20-6, AN 108-24-7  
PRO AO 934186-27-3  
CON 4 hours, 110 deg C

RX(22) RCT AO 934186-27-3, BC 934186-32-0  
RGT AX 7087-68-5 EtN(Pr-i)<sub>2</sub>, BE 358-23-6 (F<sub>3</sub>CSO<sub>2</sub>)<sub>2</sub>O  
PRO BD 934186-34-2  
SOL 75-05-8 MeCN  
CON 5 hours, -30 deg C

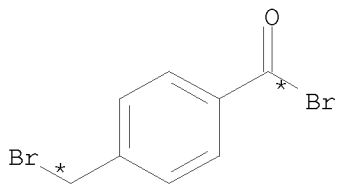
RX(133) OF 219 COMPOSED OF REACTION SEQUENCE RX(12), RX(18)  
AND REACTION SEQUENCE RX(6), RX(7), RX(8), RX(15), RX(18)

...AI + AJ ==> AK...

... Q + AN + AK ==> AS



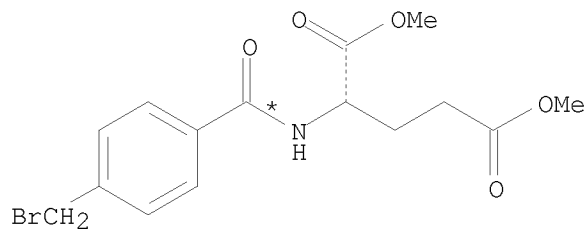
● HCl



AI

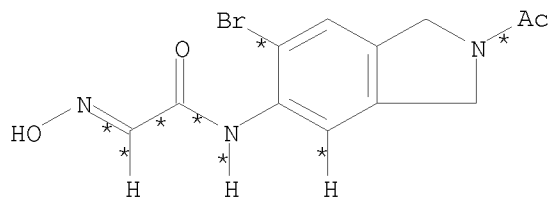
AJ

5  
STEPS  
→

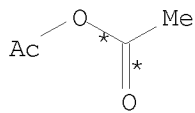


AK

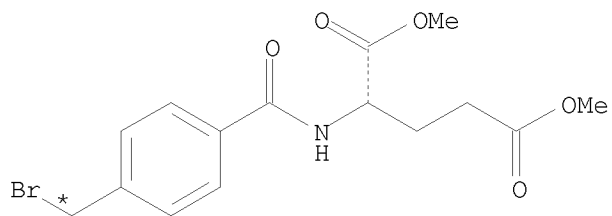
START NEXT REACTION SEQUENCE



Q

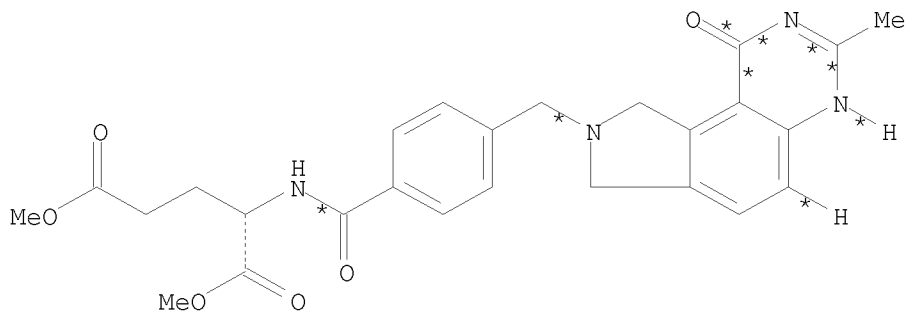


AN



AK

5  
STEPS  
→



AS  
YIELD 48%

RX(12) RCT AI 23150-65-4

STAGE (1)

RGT D 121-44-8 Et3N

SOL 75-09-2 CH2C12

CON 30 minutes, 0 deg C

STAGE (2)

RCT AJ 876-07-3

CON 1 hour, 0 deg C

PRO AK 934186-24-0

RX(6)            RCT    Q 934186-17-1  
                  RGT    H 7664-93-9 H2SO4



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PRO V 934186-18-2  
SOL 7732-18-5 Water  
CON 2 hours, 80 deg C

RX(7) RCT V 934186-18-2  
RGT X 1310-73-2 NaOH, Y 7722-84-1 H2O2  
PRO W 934186-19-3  
SOL 7732-18-5 Water  
CON 1 hour, 80 deg C

RX(8) RCT W 934186-19-3  
RGT J 1333-74-0 H2  
PRO Z 934186-20-6  
CAT 7440-05-3 Pd  
SOL 67-56-1 MeOH, 109-99-9 THF  
CON 2 hours, room temperature

RX(15) RCT Z 934186-20-6, AN 108-24-7  
PRO AO 934186-27-3  
CON 4 hours, 110 deg C

RX(18) RCT AO 934186-27-3

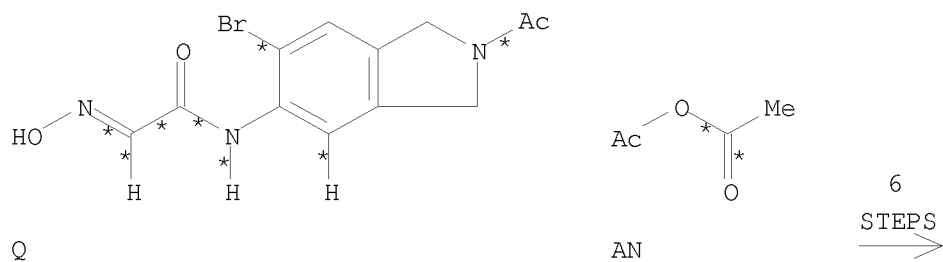
STAGE(1)  
RGT D 121-44-8 Et3N  
SOL 68-12-2 DMF  
CON 30 minutes, room temperature

STAGE(2)  
RCT AK 934186-24-0  
CON 12 hours, room temperature

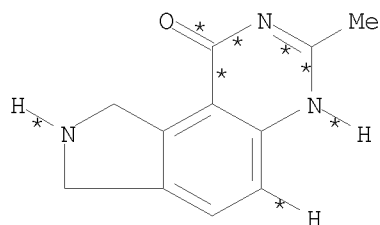
PRO AS 934186-30-8

RX(134) OF 219 COMPOSED OF RX(6), RX(7), RX(8), RX(15), RX(16), RX(17)

RX(134) Q + AN ==> AR



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● HCl

AR  
YIELD 75%

RX(6) RCT Q 934186-17-1  
RGT H 7664-93-9 H2SO4  
PRO V 934186-18-2  
SOL 7732-18-5 Water  
CON 2 hours, 80 deg C

RX(7) RCT V 934186-18-2  
RGT X 1310-73-2 NaOH, Y 7722-84-1 H2O2  
PRO W 934186-19-3  
SOL 7732-18-5 Water  
CON 1 hour, 80 deg C

RX(8) RCT W 934186-19-3  
RGT J 1333-74-0 H2  
PRO Z 934186-20-6  
CAT 7440-05-3 Pd  
SOL 67-56-1 MeOH, 109-99-9 THF  
CON 2 hours, room temperature

RX(15) RCT Z 934186-20-6, AN 108-24-7  
PRO AO 934186-27-3  
CON 4 hours, 110 deg C

RX(16) RCT AO 934186-27-3

STAGE(1)  
RGT AQ 7664-41-7 NH3  
CON 3 hours, -78 deg C

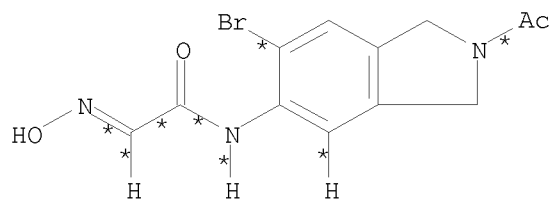
STAGE(2)  
RGT X 1310-73-2 NaOH  
SOL 7732-18-5 Water  
CON 1 hour, reflux

PRO AP 934186-28-4

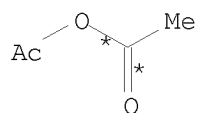
RX(17) RCT AP 934186-28-4  
RGT S 7647-01-0 HCl  
PRO AR 934186-29-5  
SOL 7732-18-5 Water  
CON 12 hours, reflux

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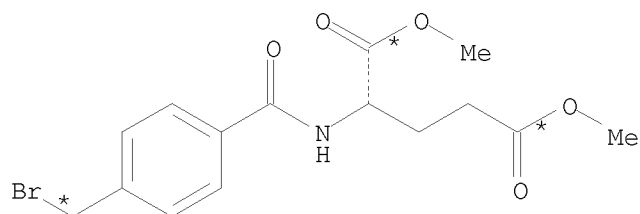
RX(135) OF 219 COMPOSED OF RX(6), RX(7), RX(8), RX(15), RX(18), RX(19)  
RX(135) Q + AN + AK ==> AT



Q

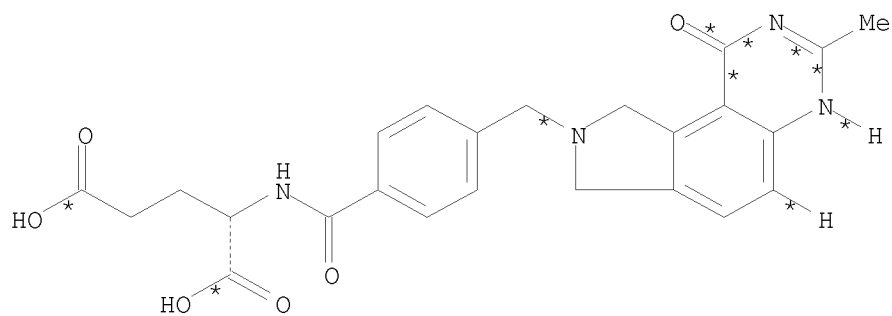


AN



AK

6  
STEPS  
→



AT  
YIELD 71%

RX(6) RCT Q 934186-17-1  
RGT H 7664-93-9 H2SO4  
PRO V 934186-18-2  
SOL 7732-18-5 Water  
CON 2 hours, 80 deg C

RX(7) RCT V 934186-18-2  
RGT X 1310-73-2 NaOH, Y 7722-84-1 H2O2  
PRO W 934186-19-3  
SOL 7732-18-5 Water  
CON 1 hour, 80 deg C

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RX(8) RCT W 934186-19-3  
RGT J 1333-74-0 H2  
PRO Z 934186-20-6  
CAT 7440-05-3 Pd  
SOL 67-56-1 MeOH, 109-99-9 THF  
CON 2 hours, room temperature

RX(15) RCT Z 934186-20-6, AN 108-24-7  
PRO AO 934186-27-3  
CON 4 hours, 110 deg C

RX(18) RCT AO 934186-27-3

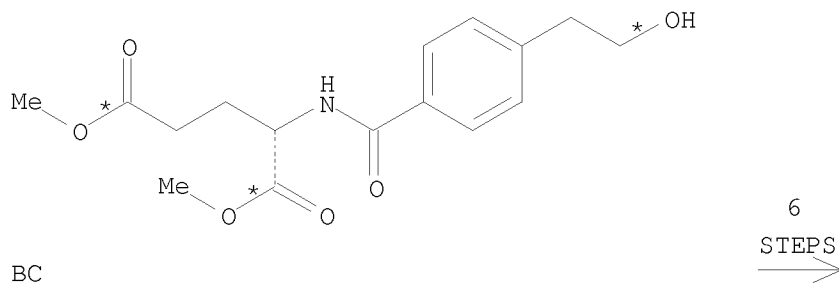
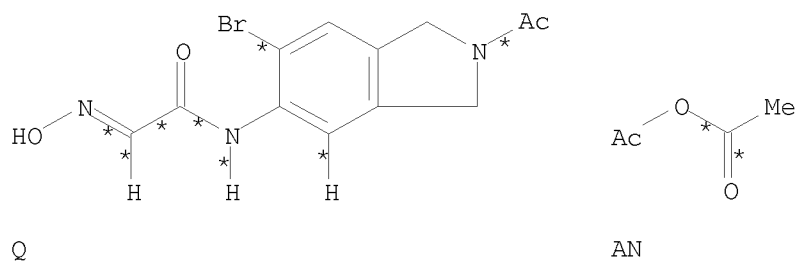
STAGE(1)  
RGT D 121-44-8 Et3N  
SOL 68-12-2 DMF  
CON 30 minutes, room temperature

STAGE(2)  
RCT AK 934186-24-0  
CON 12 hours, room temperature

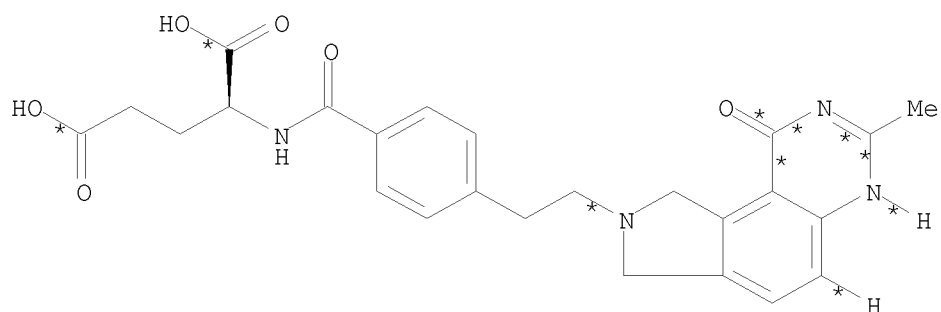
PRO AS 934186-30-8

RX(19) RCT AS 934186-30-8  
RGT X 1310-73-2 NaOH  
PRO AT 934186-26-2  
SOL 7732-18-5 Water  
CON 3 hours, 60 deg C

RX(136) OF 219 COMPOSED OF RX(6), RX(7), RX(8), RX(15), RX(22), RX(23)  
RX(136) Q + AN + BC ==> BA



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BA  
YIELD 59%

RX(6) RCT Q 934186-17-1  
RGT H 7664-93-9 H2SO4  
PRO V 934186-18-2  
SOL 7732-18-5 Water  
CON 2 hours, 80 deg C

RX(7) RCT V 934186-18-2  
RGT X 1310-73-2 NaOH, Y 7722-84-1 H2O2  
PRO W 934186-19-3  
SOL 7732-18-5 Water  
CON 1 hour, 80 deg C

RX(8) RCT W 934186-19-3  
RGT J 1333-74-0 H2  
PRO Z 934186-20-6  
CAT 7440-05-3 Pd  
SOL 67-56-1 MeOH, 109-99-9 THF  
CON 2 hours, room temperature

RX(15) RCT Z 934186-20-6, AN 108-24-7  
PRO AO 934186-27-3  
CON 4 hours, 110 deg C

RX(22) RCT AO 934186-27-3, BC 934186-32-0  
RGT AX 7087-68-5 EtN(Pr-i)2, BE 358-23-6 (F3CSO2)2O  
PRO BD 934186-34-2  
SOL 75-05-8 MeCN  
CON 5 hours, -30 deg C

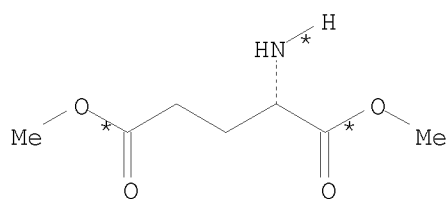
RX(23) RCT BD 934186-34-2  
RGT X 1310-73-2 NaOH  
PRO BA 934186-31-9  
SOL 7732-18-5 Water  
CON 3 hours, 60 deg C

RX(166) OF 219 COMPOSED OF REACTION SEQUENCE RX(12), RX(18), RX(19)  
AND REACTION SEQUENCE RX(6), RX(7), RX(8), RX(15), RX(18),  
RX(19)

...AI + AJ ==> AK...

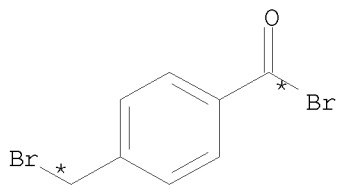
... Q + AN + AK ==> AT

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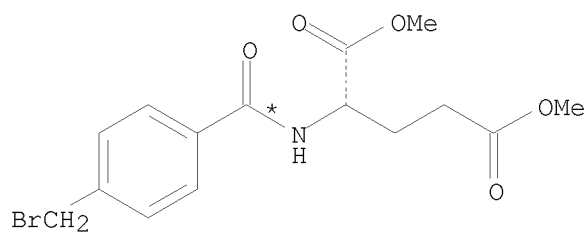
● HCl

AI



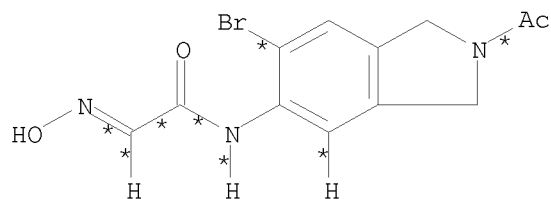
AJ

6  
STEPS  
➔

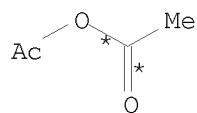


AK

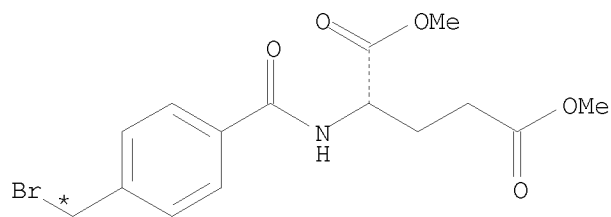
START NEXT REACTION SEQUENCE



Q



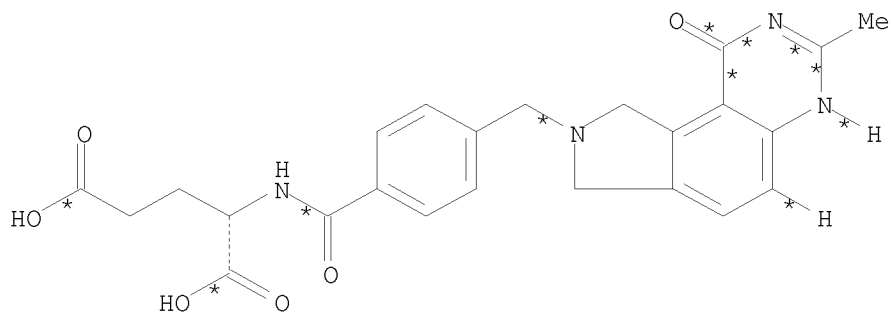
AN



AK

6  
STEPS  
➔

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AT  
YIELD 71%

RX(12) RCT AI 23150-65-4

STAGE (1)

RGT D 121-44-8 Et3N

SOL 75-09-2 CH2C12

CON 30 minutes, 0 deg C

STAGE (2)

RCT AJ 876-07-3

CON 1 hour, 0 deg C

PRO AK 934186-24-0

RX (6)	RCT	Q 934186-17-1
	RGT	H 7664-93-9 H <sub>2</sub> SO <sub>4</sub>
	PRO	V 934186-18-2
	SOL	7732-18-5 Water
	CON	2 hours, 80 deg C

```
RX(7)      RCI  V 934186-18-2
           RGT  X 1310-73-2 NaOH, Y 7722-84-1 H2O2
           PRO  W 934186-19-3
           SOL  7732-18-5 Water
           CON  1 hour, 80 deg C
```

RX (8)	RCT	W 934186-19-3
	RGT	J 1333-74-0 H2
	PRO	Z 934186-20-6
	CAT	7440-05-3 Pd
	SOL	67-56-1 MeOH, 109-99-9 THF
	CON	2 hours, room temperature

RX(15)      RCT    Z 934186-20-6, AN 108-24-7  
               PRO    AO 934186-27-3  
               CON    4 hours, 110 deg C

RX(18) RCT AO 934186-27-3

STAGE ( 1 )

RGT D 121-44-8 Et3N

SOL 68-12-2 DMF

CON 30 minutes, room temperature

STAGE(2)

RCT AK 934186-24-0  
CON 12 hours, room temperature

PRO AS 934186-30-8

RX(19) RCT AS 934186-30-8  
RGT X 1310-73-2 NaOH  
PRO AT 934186-26-2  
SOL 7732-18-5 Water  
CON 3 hours, 60 deg C

L3 ANSWER 28 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 146:337611 CASREACT

TITLE: Kynurenic acid amides as novel NR2B selective NMDA receptor antagonists

AUTHOR(S): Borza, Istvan; Kolok, Sandor; Galgoczy, Kornel; Gere, Aniko; Horvath, Csilla; Farkas, Sandor; Greiner, Istvan; Domany, Gyoergy

CORPORATE SOURCE: Gedeon Richter Ltd., H-1475, Hung.

SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(2), 406-409

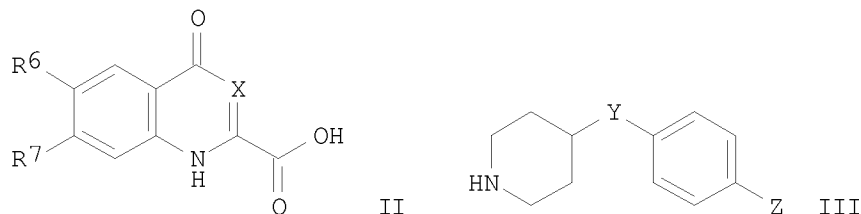
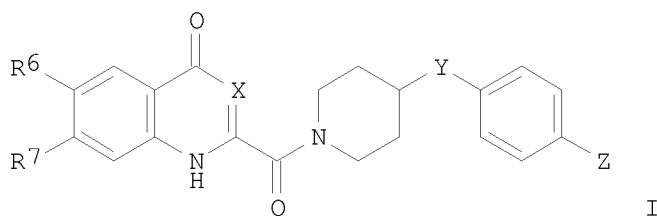
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



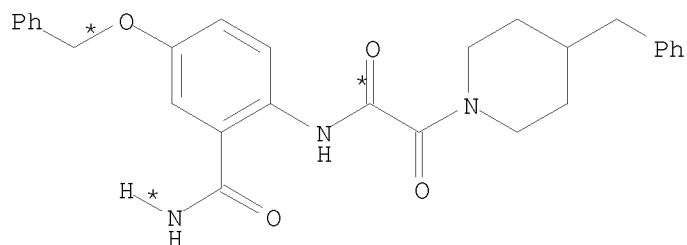
AB A novel series of kynurenic acid amides I ( $R_6 = H, OH, MeCONH$ ,  $R_7 = H, OH$ ,  $R_6R_7 = NHC(O)O$ ,  $X = CH, NH$ ,  $Y = CH_2, O$ ,  $Z = H, F, Cl, Me$ ), ring-enlarged derivs. of indole-2-carboxamides, was prepared and identified as in vivo active NR2B subtype selective NMDA receptor antagonists. The synthesis



10/ 562,112

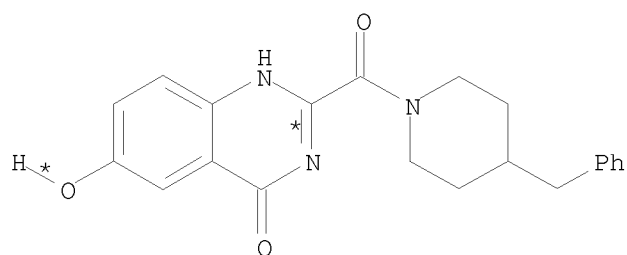
and SAR studies are discussed. The key step in the synthesis was a standard coupling reaction between and appropriately substituted kynurenic acid II and a piperidine III.

RX(27) OF 72 ...BF ==> BG



BF

(27)  
→



BG

RX(27) RCT BF 929028-80-8

STAGE(1)

CON 1.5 hours, 250 deg C

STAGE(2)

RGT N 1333-74-0 H2

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON room temperature

PRO BG 929028-81-9

NTE thermal (stage 1)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 29 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

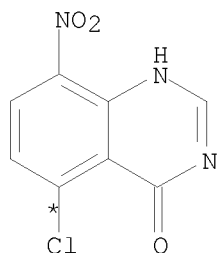
ACCESSION NUMBER: 146:45478 CASREACT

TITLE: 4'-Alkoxy substitution enhancing the anti-mitotic effect of 5-(3',4',5'-substituted)anilino-4-hydroxy-8-nitroquinazolines as a novel class of anti-microtubule

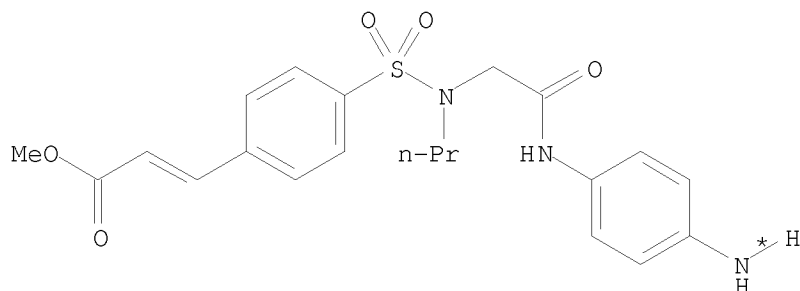
agents  
 AUTHOR(S): Jin, Yi; Zhou, Zu-Yu; Tian, Wei; Yu, Qiang; Long, Ya-Qiu  
 CORPORATE SOURCE: State Key Laboratory of Drug Research, Shanghai  
 Institute of Materia Medica, Shanghai Institutes for  
 Biological Sciences, Chinese Academy of Sciences,  
 Shanghai, 201203, Peop. Rep. China  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2006),  
 16(22), 5864-5869  
 CODEN: BMCLE8; ISSN: 0960-894X  
 PUBLISHER: Elsevier Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Mitosis inhibitors are powerful anticancer drugs. Based on a novel anti-microtubule agent 5-(4'-methoxy)anilino-4-hydroxy-8-nitroquinazoline, a series of 5-(3',4',5'-substituted)anilino-4-hydroxy-8-nitroquinazolines were designed and synthesized to investigate the effect of the substitution on the inhibitory activity against mitotic progression of tumor cells. The large alkoxy substitution on the 4'-position of 5-anilino ring is beneficial for the potency. The 5-(3',4',5'-trimethoxy)anilino-8-nitroquinazoline (1h) displays an overwhelming activity in arresting the cells at the G2/M phase, providing a promising new template for further development of potent microtubule-targeted anti-mitotic drugs.

RX(35) OF 146 ...CB + AY ==> CG



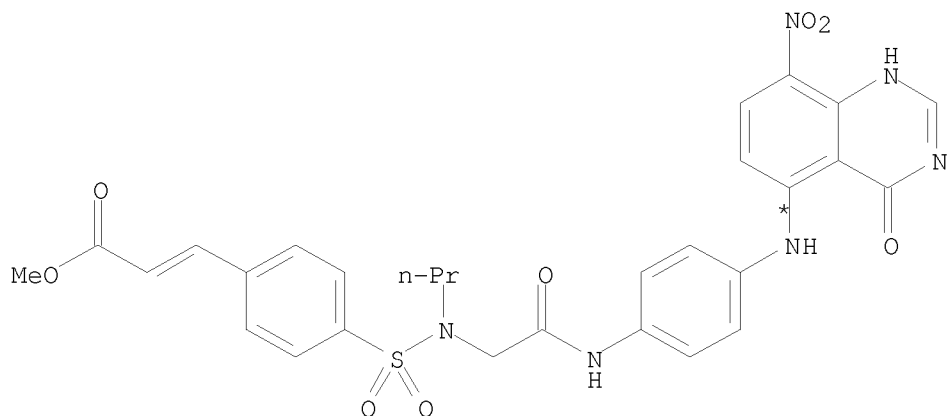
CB



AY

(35)  $\longrightarrow$

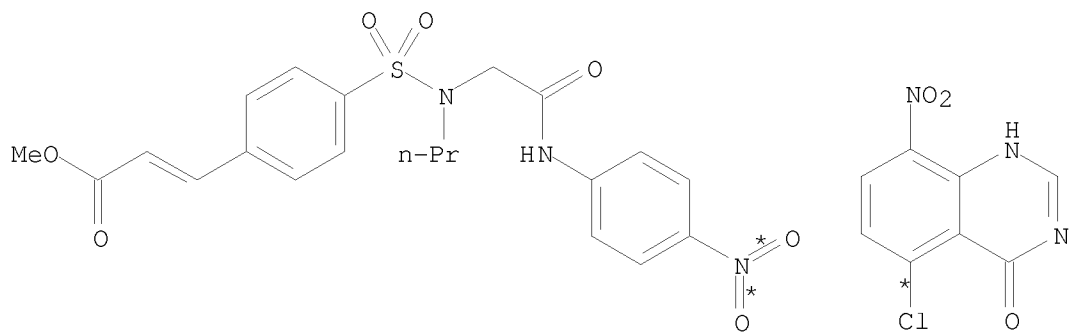
10/ 562,112



CG  
YIELD 80%

RX(35)     RCT    CB 400784-50-1, AY 916336-22-6  
          RGT    AN 7087-68-5 EtN(Pr-i)2  
          PRO    CG 916336-26-0  
          SOL    109-99-9 THF  
          CON    12 - 24 hours, reflux

RX(57) OF 146 COMPOSED OF RX(19), RX(35)  
RX(57)     AP   +   CB   ==>   CG

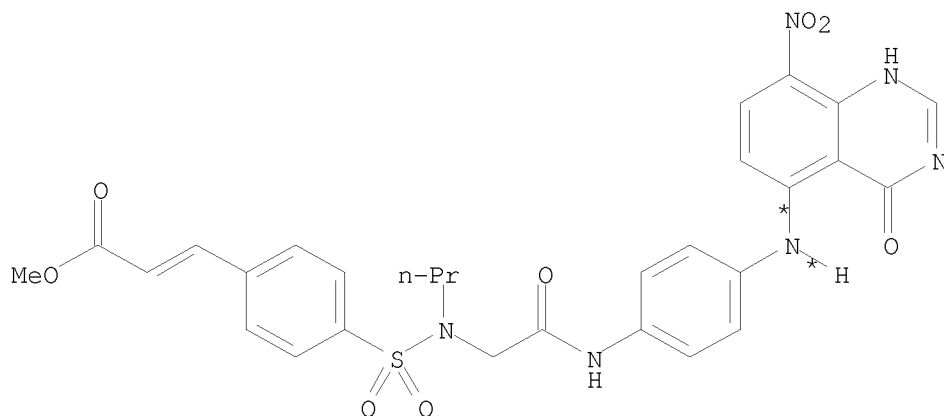


AP

CB

2  
STEPS  
→

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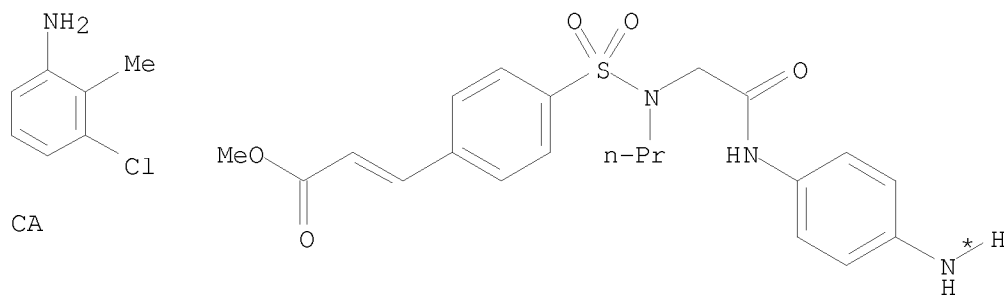


CG  
YIELD 80%

RX(19) RCT AP 916336-31-7  
RGT O 12125-02-9 NH4Cl, P 7439-89-6 Fe  
PRO AY 916336-22-6  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON reflux

RX(35) RCT CB 400784-50-1, AY 916336-22-6  
RGT AN 7087-68-5 EtN(Pr-i)2  
PRO CG 916336-26-0  
SOL 109-99-9 THF  
CON 12 - 24 hours, reflux

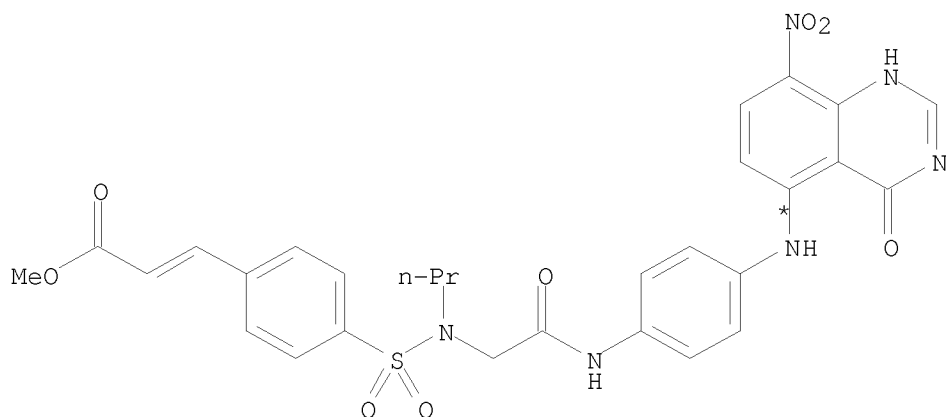
RX(72) OF 146 COMPOSED OF RX(30), RX(35)  
RX(72) CA + AY ==> CG



AY

2  
STEPS  
→

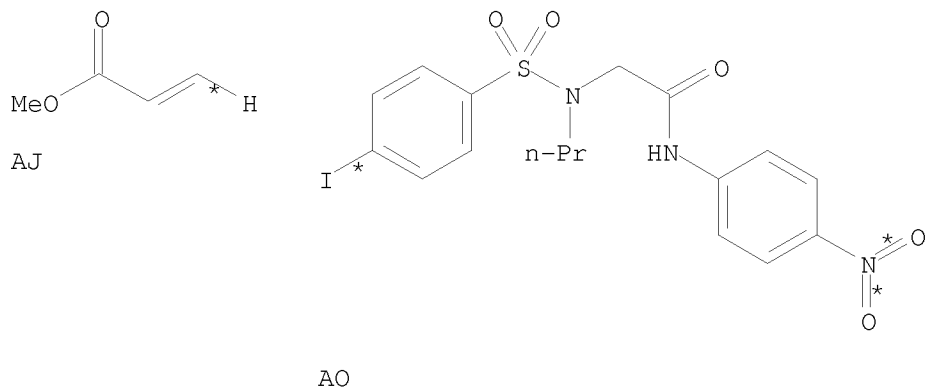
10/ 562,112



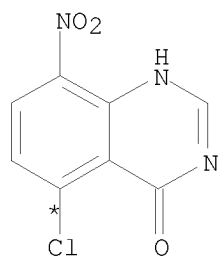
CG  
YIELD 80%

RX(30)	RCT	CA 87-60-5
	PRO	CB 400784-50-1
	NTE	no experimental detail
RX(35)	RCT	CB 400784-50-1, AY 916336-22-6
	RGT	AN 7087-68-5 EtN(Pr-i) <sub>2</sub>
	PRO	CG 916336-26-0
	SOL	109-99-9 THF
	CON	12 - 24 hours, reflux

RX(98) OF 146 COMPOSED OF RX(14), RX(19), RX(35)  
RX(98) AJ + AO + CB ==> CG

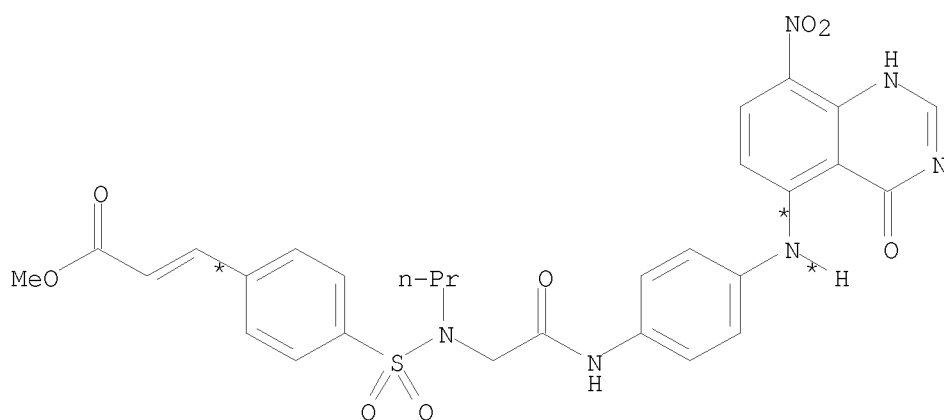


10/ 562,112



CB

3  
STEPS  
→



CG

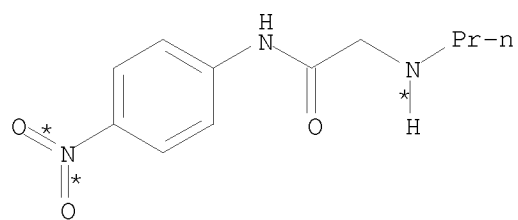
YIELD 80%

RX(14) RCT AJ 96-33-3, AO 916336-34-0  
RGT AL 7699-45-8 ZnBr<sub>2</sub>  
PRO AP 916336-31-7  
CAT 13965-03-2 PdCl<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub>  
SOL 109-99-9 THF, 7087-68-5 EtN(Pr-i)<sub>2</sub>  
CON room temperature

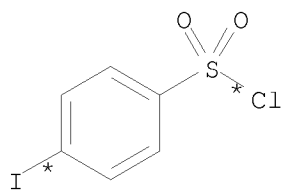
RX(19) RCT AP 916336-31-7  
RGT O 12125-02-9 NH<sub>4</sub>Cl, P 7439-89-6 Fe  
PRO AY 916336-22-6  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON reflux

RX(35) RCT CB 400784-50-1, AY 916336-22-6  
RGT AN 7087-68-5 EtN(Pr-i)<sub>2</sub>  
PRO CG 916336-26-0  
SOL 109-99-9 THF  
CON 12 - 24 hours, reflux

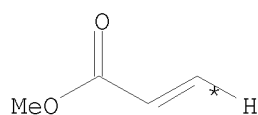
RX(99) OF 146 COMPOSED OF RX(18), RX(14), RX(19), RX(35)  
RX(99) AW + AX + AJ + CB ==> CG



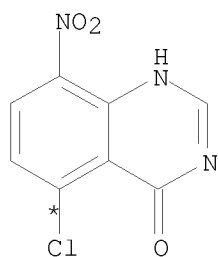
AW



AX

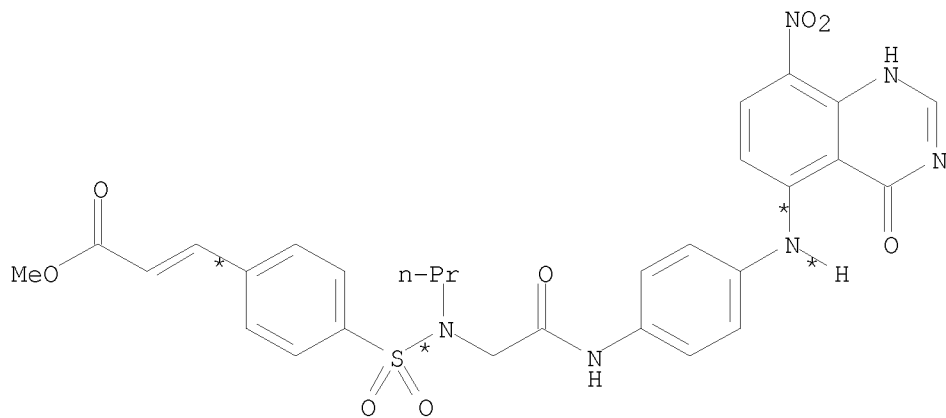


AJ



CB

4  
STEPS  
→



CG

YIELD 80%

RX(18) RCT AW 699532-45-1, AX 98-61-3  
RGT AN 7087-68-5 EtN(Pr-i)<sub>2</sub>  
PRO AO 916336-34-0  
SOL 109-99-9 THF  
CON room temperature

RX(14) RCT AJ 96-33-3, AO 916336-34-0  
RGT AL 7699-45-8 ZnBr<sub>2</sub>  
PRO AP 916336-31-7  
CAT 13965-03-2 PdCl<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub>

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SOL 109-99-9 THF, 7087-68-5 EtN(Pr-i)2  
CON room temperature

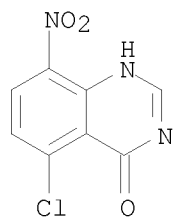
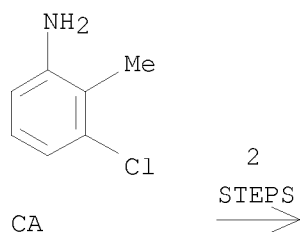
RX(19) RCT AP 916336-31-7  
RGT O 12125-02-9 NH4Cl, P 7439-89-6 Fe  
PRO AY 916336-22-6  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON reflux

RX(35) RCT CB 400784-50-1, AY 916336-22-6  
RGT AN 7087-68-5 EtN(Pr-i)2  
PRO CG 916336-26-0  
SOL 109-99-9 THF  
CON 12 - 24 hours, reflux

RX(107) OF 146 COMPOSED OF REACTION SEQUENCE RX(30), RX(35)  
AND REACTION SEQUENCE RX(19), RX(35)

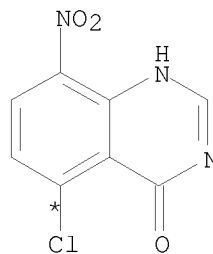
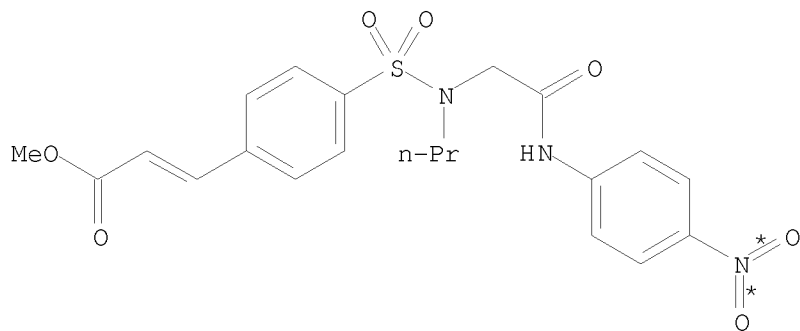
...CA ==> CB...

... AP + CB ==> CG



CB

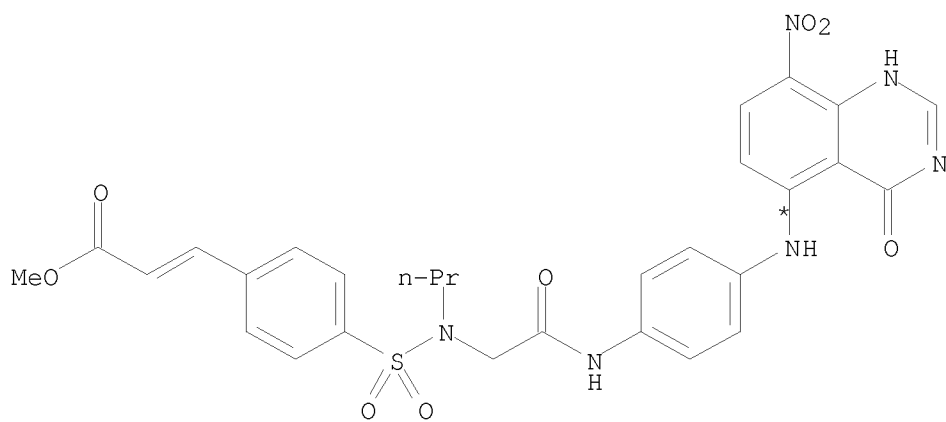
START NEXT REACTION SEQUENCE





10/ 562,112

2  
STEPS  
→

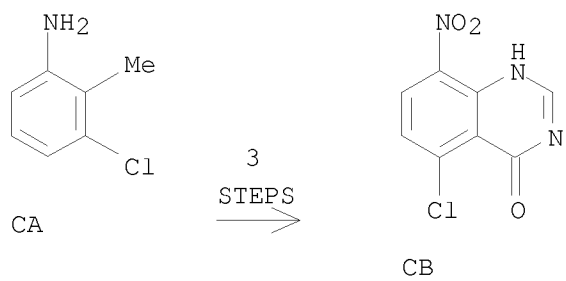


CG  
YIELD 80%

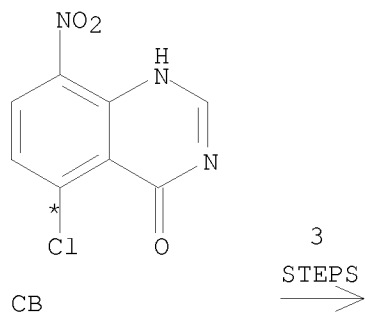
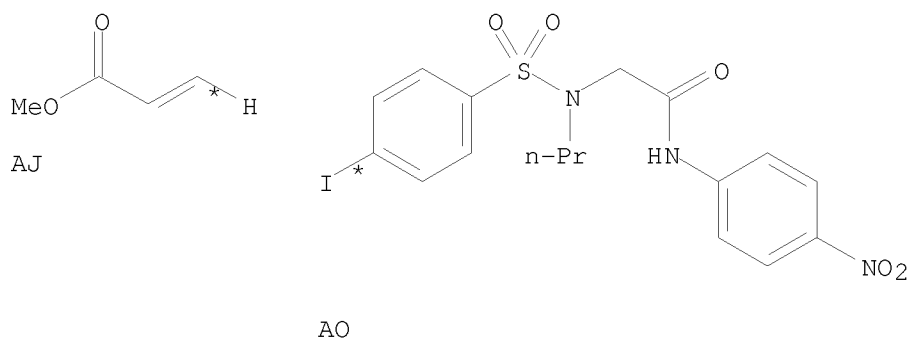
RX(30)	RCT	CA 87-60-5
	PRO	CB 400784-50-1
	NTE	no experimental detail
RX(19)	RCT	AP 916336-31-7
	RGT	O 12125-02-9 NH <sub>4</sub> Cl, P 7439-89-6 Fe
	PRO	AY 916336-22-6
	SOL	7732-18-5 Water, 67-56-1 MeOH
	CON	reflux
RX(35)	RCT	CB 400784-50-1, AY 916336-22-6
	RGT	AN 7087-68-5 EtN(Pr-i) <sub>2</sub>
	PRO	CG 916336-26-0
	SOL	109-99-9 THF
	CON	12 - 24 hours, reflux

RX(108) OF 146 COMPOSED OF REACTION SEQUENCE RX(30), RX(35)  
AND REACTION SEQUENCE RX(14), RX(19), RX(35)

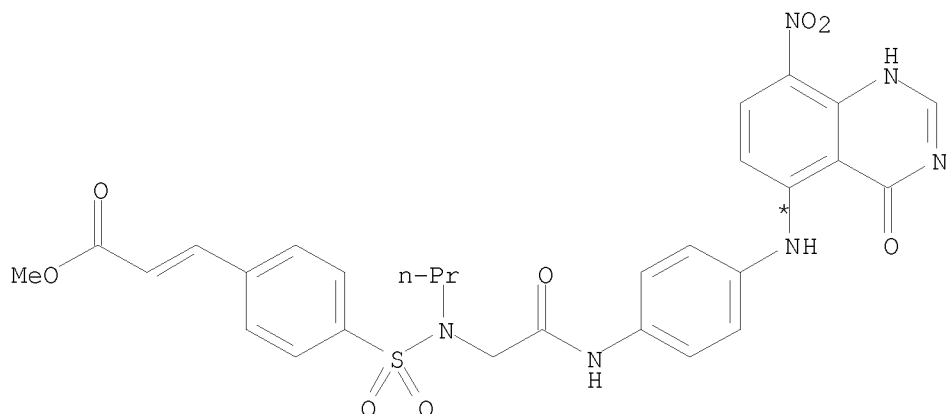
...CA ==> CB...  
...AJ + AO + CB ==> CG



START NEXT REACTION SEQUENCE



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CG  
YIELD 80%

RX(30) RCT CA 87-60-5  
PRO CB 400784-50-1  
NTE no experimental detail

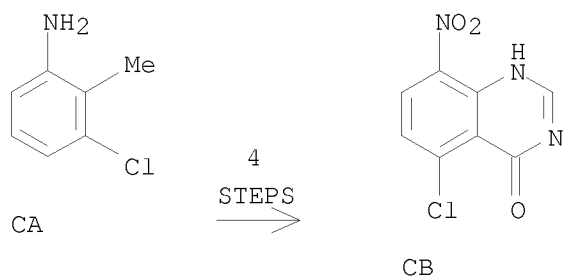
RX(14) RCT AJ 96-33-3, AO 916336-34-0  
RGT AL 7699-45-8 ZnBr2  
PRO AP 916336-31-7  
CAT 13965-03-2 PdCl2(PPh3)2  
SOL 109-99-9 THF, 7087-68-5 EtN(Pr-i)2  
CON room temperature

RX(19) RCT AP 916336-31-7  
RGT O 12125-02-9 NH4Cl, P 7439-89-6 Fe  
PRO AY 916336-22-6  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON reflux

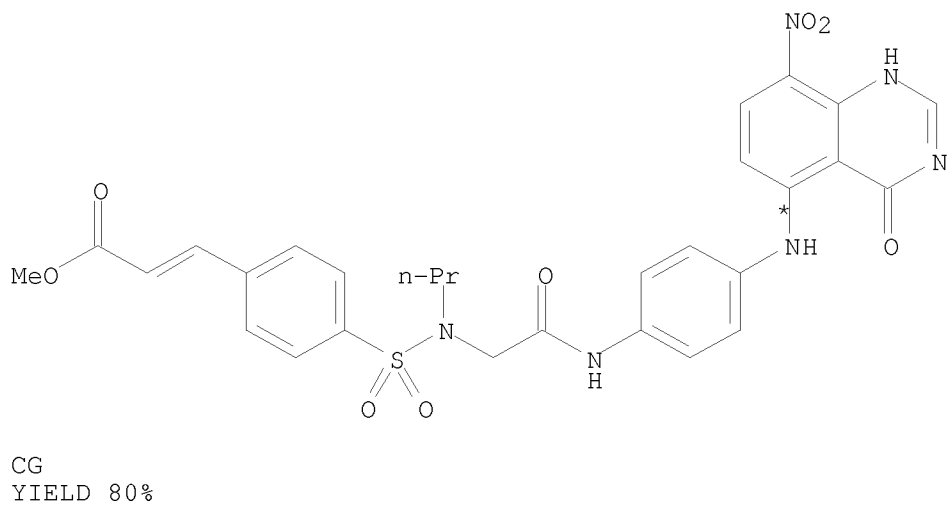
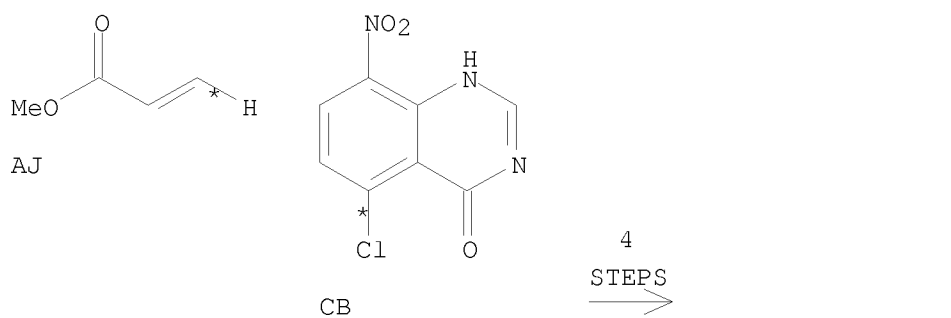
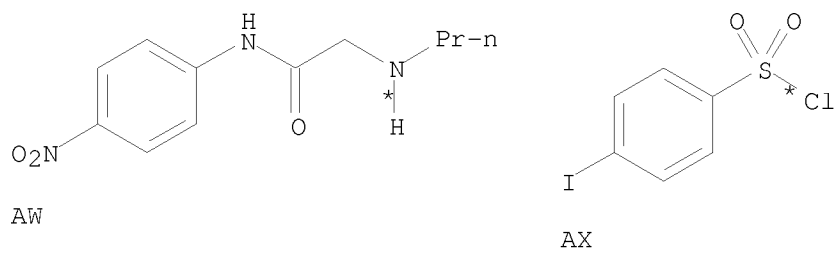
RX(35) RCT CB 400784-50-1, AY 916336-22-6  
RGT AN 7087-68-5 EtN(Pr-i)2  
PRO CG 916336-26-0  
SOL 109-99-9 THF  
CON 12 - 24 hours, reflux

RX(135) OF 146 COMPOSED OF REACTION SEQUENCE RX(30), RX(35)  
AND REACTION SEQUENCE RX(18), RX(14), RX(19), RX(35)  
...CA ==> CB...  
... AW + AX + AJ + CB ==> CG

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START NEXT REACTION SEQUENCE

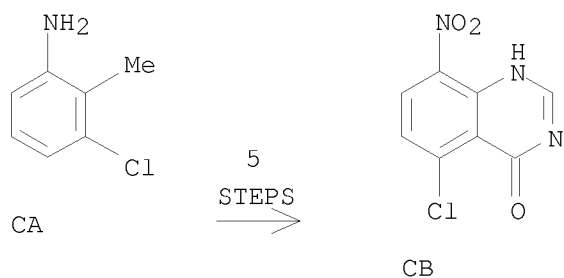


RX(30)     RCT   CA 87-60-5  
              PRO   CB 400784-50-1  
              NTE   no experimental detail  
  
 RX(18)     RCT   AW 699532-45-1, AX 98-61-3  
              RGT   AN 7087-68-5 EtN(Pr-i)2  
              PRO   AO 916336-34-0  
              SOL   109-99-9 THF  
              CON   room temperature  
  
 RX(14)     RCT   AJ 96-33-3, AO 916336-34-0  
              RGT   AL 7699-45-8 ZnBr2  
              PRO   AP 916336-31-7  
              CAT   13965-03-2 PdCl2(PPh3)2  
              SOL   109-99-9 THF, 7087-68-5 EtN(Pr-i)2  
              CON   room temperature  
  
 RX(19)     RCT   AP 916336-31-7  
              RGT   O 12125-02-9 NH4Cl, P 7439-89-6 Fe  
              PRO   AY 916336-22-6  
              SOL   7732-18-5 Water, 67-56-1 MeOH  
              CON   reflux  
  
 RX(35)     RCT   CB 400784-50-1, AY 916336-22-6  
              RGT   AN 7087-68-5 EtN(Pr-i)2  
              PRO   CG 916336-26-0  
              SOL   109-99-9 THF  
              CON   12 - 24 hours, reflux

RX(136) OF 146 COMPOSED OF REACTION SEQUENCE RX(30), RX(35)  
 AND REACTION SEQUENCE RX(17), RX(18), RX(14), RX(19), RX(35)

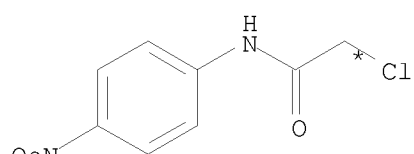
...CA ==> CB...

... AT + AV + AX + AJ + CB ==> CG

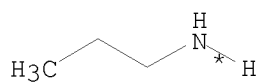


START NEXT REACTION SEQUENCE

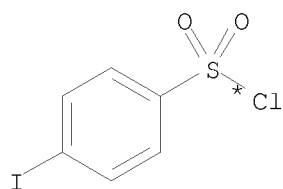
10/ 562,112



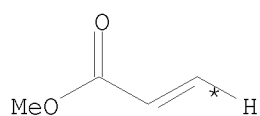
AT



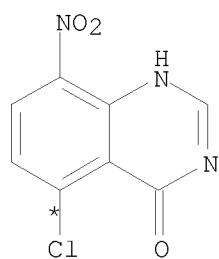
AV



AX

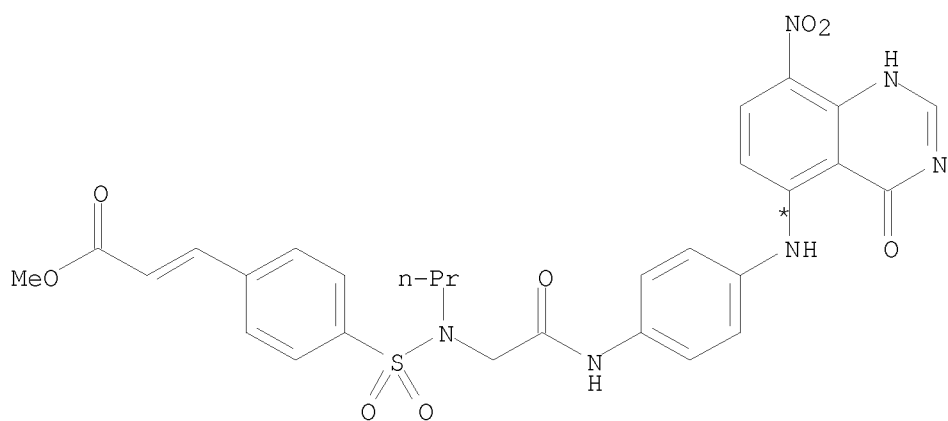


AJ



CB

5  
STEPS  
→



CG

YIELD 80%

RX(30)

RCT

CA 87-60-5

PRO

CB 400784-50-1

NTE no experimental detail

RX(17) RCT AT 17329-87-2, AV 107-10-8  
 PRO AW 699532-45-1  
 SOL 109-99-9 THF  
 CON room temperature

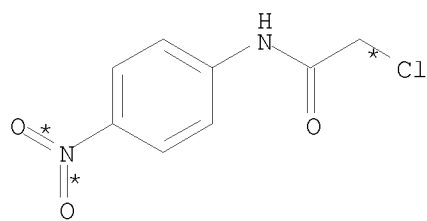
RX(18) RCT AW 699532-45-1, AX 98-61-3  
 RGT AN 7087-68-5 EtN(Pr-i)2  
 PRO AO 916336-34-0  
 SOL 109-99-9 THF  
 CON room temperature

RX(14) RCT AJ 96-33-3, AO 916336-34-0  
 RGT AL 7699-45-8 ZnBr2  
 PRO AP 916336-31-7  
 CAT 13965-03-2 PdCl2(PPh3)2  
 SOL 109-99-9 THF, 7087-68-5 EtN(Pr-i)2  
 CON room temperature

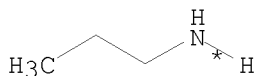
RX(19) RCT AP 916336-31-7  
 RGT O 12125-02-9 NH4Cl, P 7439-89-6 Fe  
 PRO AY 916336-22-6  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON reflux

RX(35) RCT CB 400784-50-1, AY 916336-22-6  
 RGT AN 7087-68-5 EtN(Pr-i)2  
 PRO CG 916336-26-0  
 SOL 109-99-9 THF  
 CON 12 - 24 hours, reflux

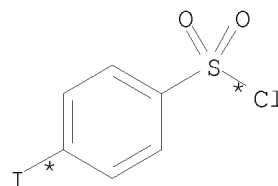
RX(139) OF 146 COMPOSED OF RX(17), RX(18), RX(14), RX(19), RX(35)  
 RX(139) AT + AV + AX + AJ + CB ==> CG



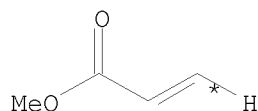
AT



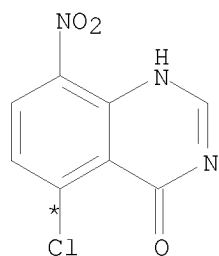
AV



AX

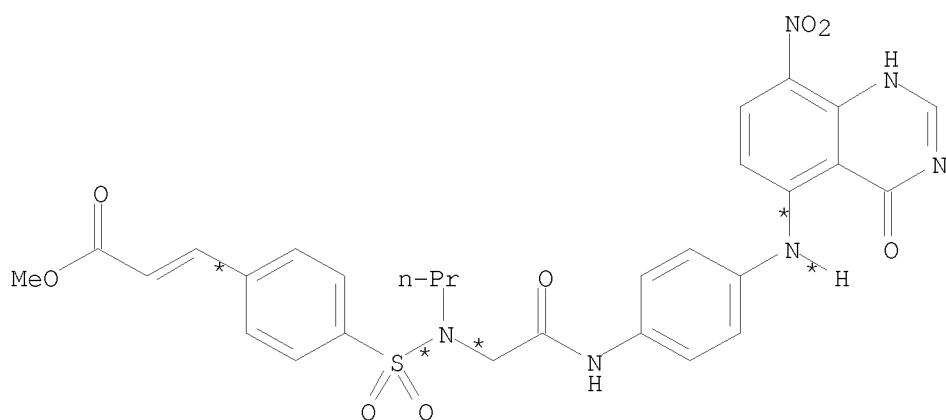


AJ



CB

5  
STEPS  
→



CG

YIELD 80%

- |        |     |   |
|--------|-----|---|
| RX(17) | RCT | AT 17329-87-2, AV 107-10-8                                    |
|        | PRO | AW 699532-45-1  |
|        | SOL | 109-99-9 THF  |
|        | CON | room temperature  |
| RX(18) | RCT | AW 699532-45-1, AX 98-61-3                                    |
|        | RGT | AN 7087-68-5 EtN(Pr-i) <sub>2</sub>                           |
|        | PRO | AO 916336-34-0  |
|        | SOL | 109-99-9 THF  |
|        | CON | room temperature  |
| RX(14) | RCT | AJ 96-33-3, AO 916336-34-0                                    |
|        | RGT | AL 7699-45-8 ZnBr <sub>2</sub>                                |
|        | PRO | AP 916336-31-7  |
|        | CAT | 13965-03-2 PdCl <sub>2</sub> (PPh <sub>3</sub> ) <sub>2</sub> |
|        | SOL | 109-99-9 THF, 7087-68-5 EtN(Pr-i) <sub>2</sub>                |
|        | CON | room temperature  |
| RX(19) | RCT | AP 916336-31-7  |
|        | RGT | O 12125-02-9 NH <sub>4</sub> Cl, P 7439-89-6 Fe               |
|        | PRO | AY 916336-22-6  |
|        | SOL | 7732-18-5 Water, 67-56-1 MeOH                                 |
|        | CON | reflux  |

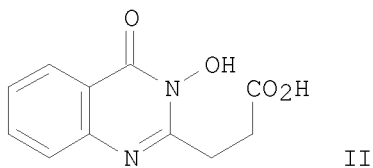
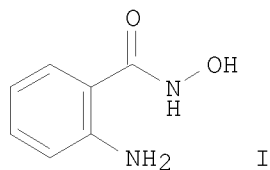


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RX(35) RCT CB 400784-50-1, AY 916336-22-6  
RGT AN 7087-68-5 EtN(Pr-i)2  
PRO CG 916336-26-0  
SOL 109-99-9 THF  
CON 12 - 24 hours, reflux

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

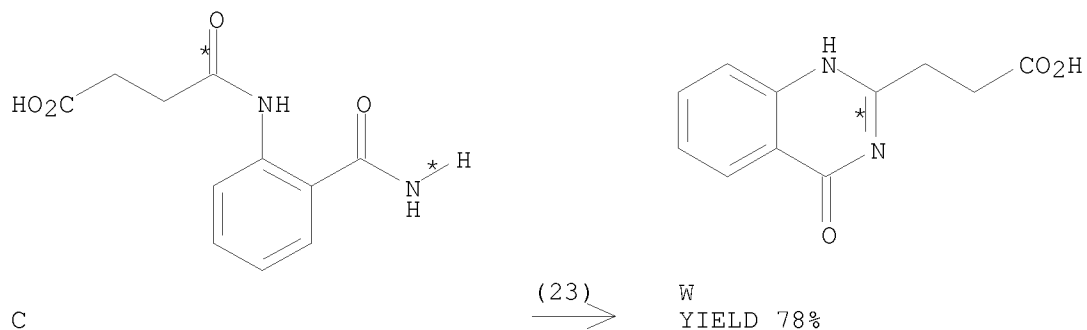
L3 ANSWER 30 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 145:505395 CASREACT  
TITLE: Reaction of anthranilic acid amides with cyclic  
anhydrides  
AUTHOR(S): Shemchuk, L. A.; Chernykh, V. P.; Krys'kiv, O. S.  
CORPORATE SOURCE: National Pharmaceutical University, Kharkov, 61002,  
Ukraine  
SOURCE: Russian Journal of Organic Chemistry (2006), 42(3),  
382-387  
CODEN: RJOCEQ; ISSN: 1070-4280  
PUBLISHER: Pleiades Publishing, Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Anthranilic acid amide reacts with cyclic anhydrides to give the  
corresponding N-acyl derivs. at the amino group, while analogous reactions  
of o-aminobenzohydroxamic acid (I) lead to formation of  
3-hydroxy-quinazolin-4-ones, e.g., II, under mild conditions. N-Acyl  
derivs. of anthranilic acid amide undergo intramol. cyclization to imides  
on microwave irradiation or on melting, and their treatment with acetic  
anhydride in the presence of sodium acetate on heating yields  
quinazolin-4-ones.

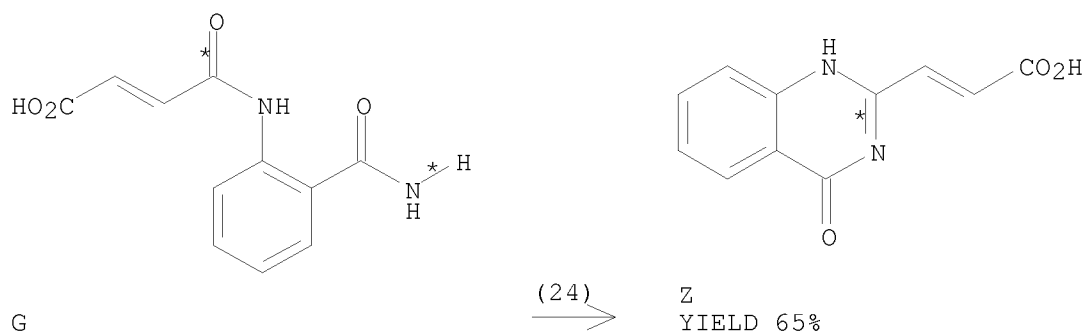
RX(23) OF 56 ...C ==> W...

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RX(23)    RCT   C 306325-56-4  
           RGT   X 127-09-3 AcONa  
           PRO   W 5368-37-6  
           SOL   108-24-7 Ac2O  
           CON   SUBSTAGE(1) 15 minutes, reflux  
                      SUBSTAGE(2) cooled  
           NTE   products depend on reaction conditions

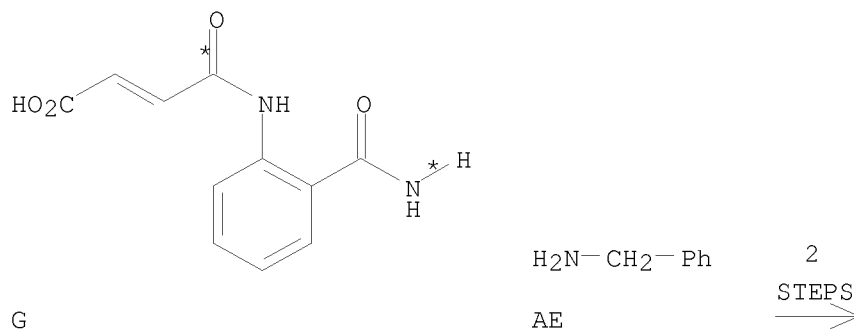
RX(24) OF 56    ...G ==> Z...



RX(24)    RCT   G 303770-83-4  
           RGT   X 127-09-3 AcONa  
           PRO   Z 5584-96-3  
           SOL   108-24-7 Ac2O  
           CON   SUBSTAGE(1) 15 minutes, reflux  
                      SUBSTAGE(2) cooled  
           NTE   products depend on reaction conditions

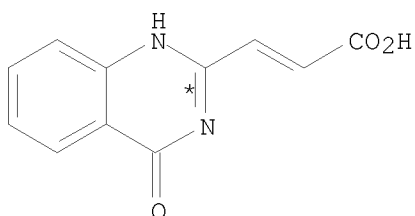
RX(51) OF 56 COMPOSED OF RX(23), RX(30)  
 RX(51)    C + AE ==> AF





H<sub>2</sub>N-CH<sub>2</sub>-Ph

AH: CM 1  
YIELD 65%



AH: CM 2  
YIELD 65%

RX(24) RCT G 303770-83-4  
 RGT X 127-09-3 AcONa  
 PRO Z 5584-96-3  
 SOL 108-24-7 Ac2O  
 CON SUBSTAGE(1) 15 minutes, reflux  
 SUBSTAGE(2) cooled  
 NTE products depend on reaction conditions

RX(31) RCT Z 5584-96-3, AE 100-46-9  
 PRO AH 915215-80-4  
 SOL 64-17-5 EtOH  
 CON 30 minutes, room temperature  
 NTE using dioxane as solvent gave same result

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

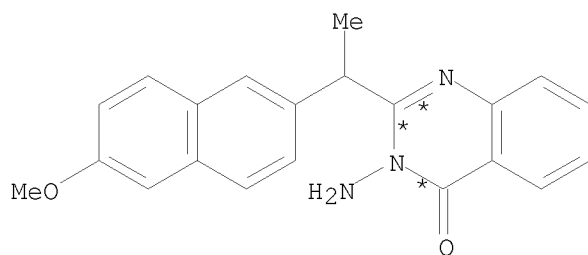
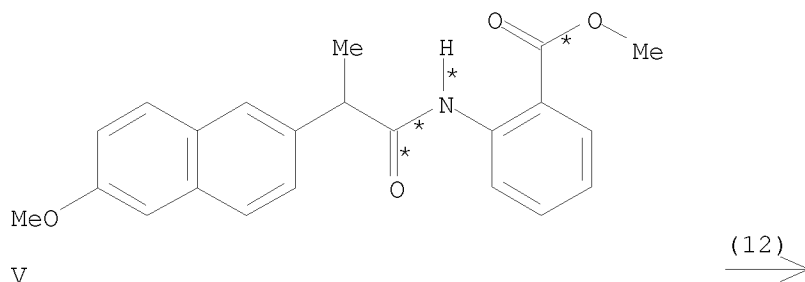
L3 ANSWER 31 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 145:489192 CASREACT  
 TITLE: Propionic acids in organic synthesis: novel synthesis of benzimidazole, 3,1-benzoxazine, 3-aminoquinazoline and 3-aminothieno[2,3-d]pyrimidine derivatives containing 2-naphthyl propionyl moiety  
 AUTHOR(S): Al-Sehemi, Abdullah G. M.; El-Sharief, A. M. Sh; Ammar, Y. A.  
 CORPORATE SOURCE: Chemistry Department, Teacher's College, Abha, Saudi

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SOURCE: Arabia  
Indian Journal of Chemistry, Section B: Organic  
Chemistry Including Medicinal Chemistry (2006),  
45B(2), 450-455  
CODEN: IJSBDB; ISSN: 0376-4699  
PUBLISHER: National Institute of Science Communication and  
Information Resources  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Naproxenoyl chloride (I) is reacted with  $\text{NH}_4\text{SCN}$  and  $\text{NaN}_3$  to produce the acid isothiocyanate and acid azide, resp. Interaction of the isothiocyanate with 1,2-phenylenediamine and anthranilic acid produced the corresponding benzimidazole 5 and 3,1-benzoxazine, resp. Treatment of the acid azide with 4-toluidine afforded the corresponding urea derivative. A novel quinazolinone is synthesized by acylation of Me anthranilate with I followed by treatment with  $\text{N}_2\text{H}_4 \cdot \text{H}_2\text{O}$ .

RX(12) OF 65 ...V ==> AA...

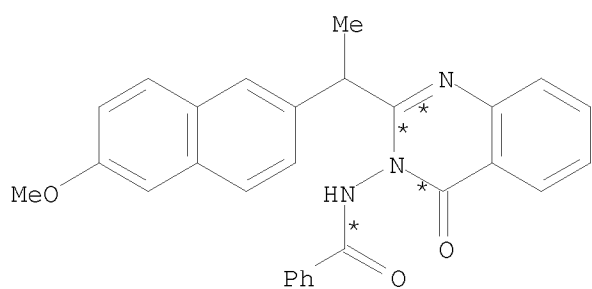
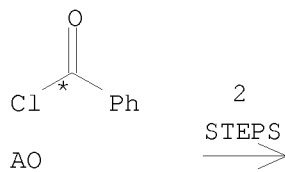
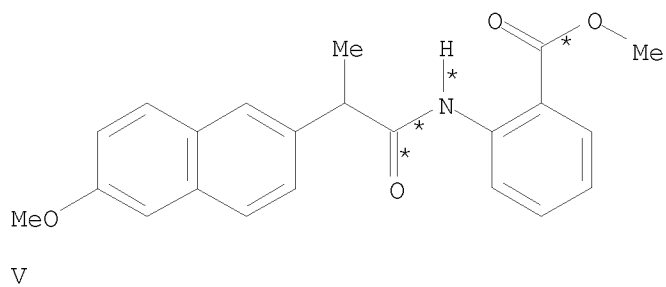


YIELD 65%

RX(12) RCT V 177585-58-9  
RGT AB 7803-57-8  $\text{N}_2\text{H}_4 \cdot \text{H}_2\text{O}$   
PRO AA 354786-03-1  
SOL 71-36-3 BuOH  
CON 10 hours, reflux

RX(42) OF 65 COMPOSED OF RX(12), RX(20)  
RX(42) V + AO ==> AP

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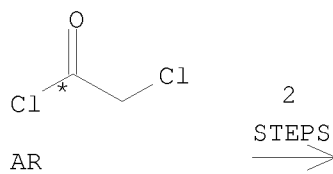
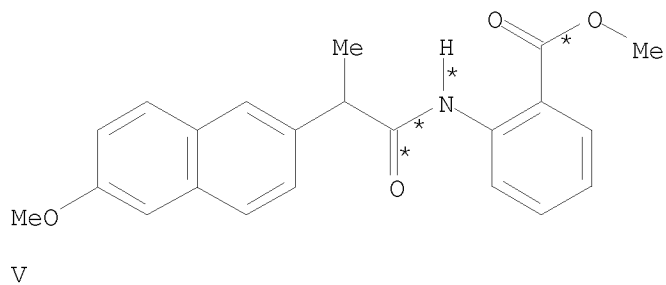
YIELD 60%

RX(12) RCT V 177585-58-9  
RGT AB 7803-57-8 N2H4-H2O  
PRO AA 354786-03-1  
SOL 71-36-3 BuOH  
CON 10 hours, reflux

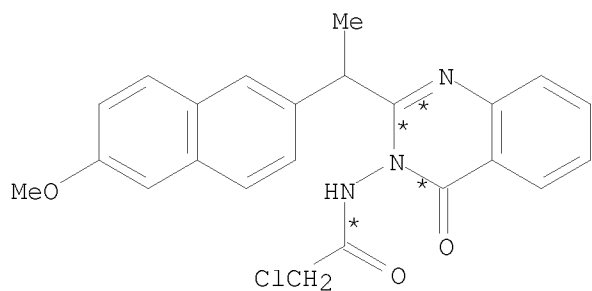
RX(20) RCT AA 354786-03-1, AO 98-88-4  
RGT AQ 110-86-1 Pyridine  
PRO AP 914398-10-0  
SOL 110-86-1 Pyridine  
CON 1 hour, reflux

RX(43) OF 65 COMPOSED OF RX(12), RX(21)

RX(43) V + AR ==> AS



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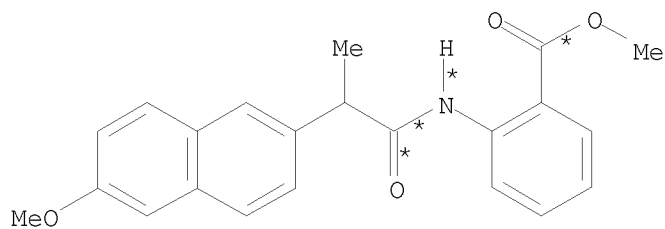


AS  
YIELD 62%

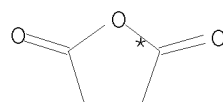
RX(12)     RCT    V 177585-58-9  
             RGT    AB 7803-57-8 N2H4-H2O  
             PRO    AA 354786-03-1  
             SOL    71-36-3 BuOH  
             CON    10 hours, reflux

RX(21)     RCT    AA 354786-03-1, AR 79-04-9  
             RGT    AQ 110-86-1 Pyridine  
             PRO    AS 914398-11-1  
             SOL    110-86-1 Pyridine  
             CON    1 hour, reflux

RX(44) OF 65 COMPOSED OF RX(12), RX(22)  
RX(44)     V   +   AT   ==>   AU



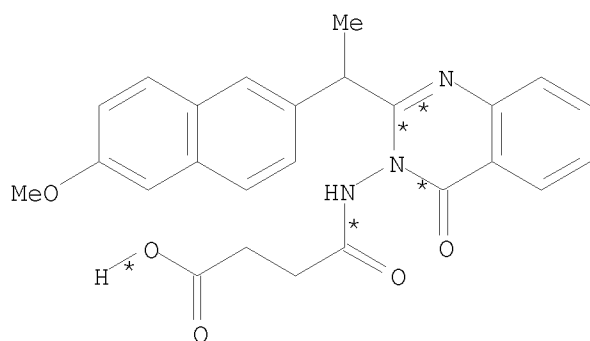
V



AT

2  
STEPS  
→

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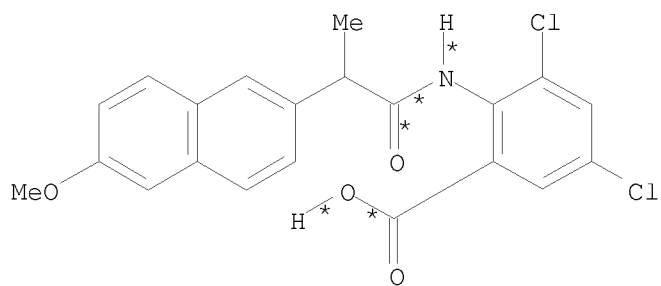


AU  
YIELD 60%

RX(12) RCT V 177585-58-9  
RGT AB 7803-57-8 N2H4-H2O  
PRO AA 354786-03-1  
SOL 71-36-3 BuOH  
CON 10 hours, reflux

RX(22) RCT AA 354786-03-1, AT 108-30-5  
PRO AU 914398-12-2  
SOL 64-17-5 EtOH  
CON 3 hours, reflux

RX(45) OF 65 COMPOSED OF RX(14), RX(15)  
RX(45) Z ==> AG

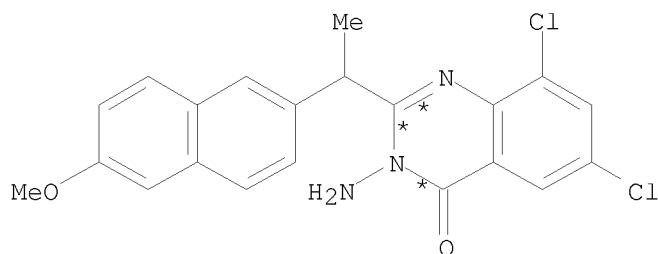


Z

2  
STEPS  
→



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AG  
YIELD 62%

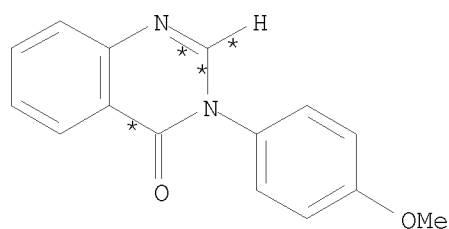
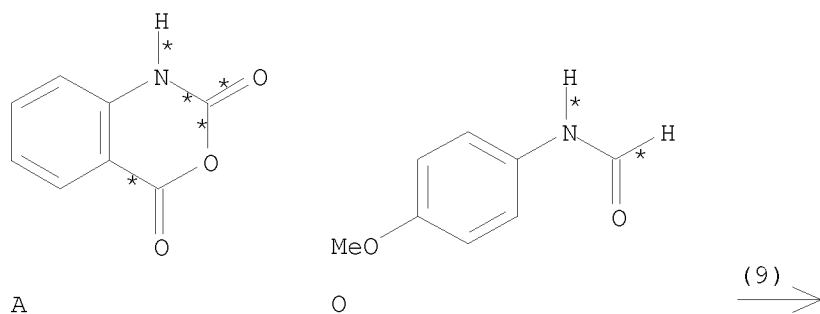
RX(14) RCT Z 914398-03-1  
RGT AE 108-24-7 Ac2O  
PRO AF 914398-05-3  
SOL 108-24-7 Ac2O  
CON 5 hours, reflux

RX(15) RCT AF 914398-05-3  
RGT AB 7803-57-8 N2H4-H2O  
PRO AG 914398-22-4  
SOL 64-17-5 EtOH  
CON 24 hours, reflux

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 32 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 145:271726 CASREACT  
TITLE: Convergent one-pot synthesis of 3-substituted  
quinazolin-4(3H)-ones under solvent-free conditions  
AUTHOR(S): Samavi, Laleh  
CORPORATE SOURCE: Department of Chemistry, Guilan University, Rasht,  
Iran  
SOURCE: Synthetic Communications (2006), 36(15), 2245-2252  
CODEN: SYNCAV; ISSN: 0039-7911  
PUBLISHER: Taylor & Francis, Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB A convenient method for the synthesis of 3-substituted  
quinazolin-4(3H)-ones using the convergent reactions of formic acid, a  
primary amine, and isatoic anhydride under solvent-free conditions and  
with brief microwave irradiation is described.

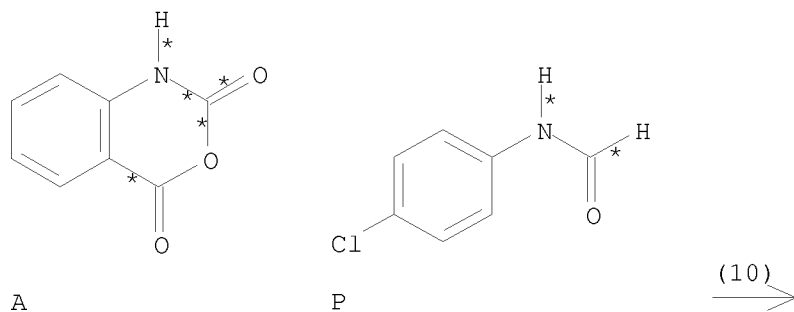
RX(9) OF 18 ...A + O ==> L



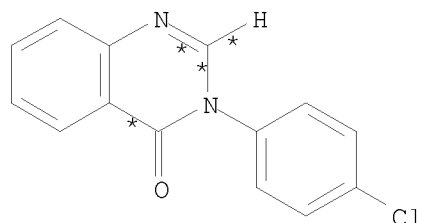
L  
YIELD 62%

RX(9) RCT A 118-48-9, O 5470-34-8  
 PRO L 22378-45-6  
 CON 6 minutes, heated  
 NTE a few drops of DMF used, green chemistry-solvent, microwave irradiation, no solvent

RX(10) OF 18 ...A + P ==> N



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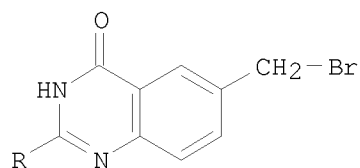


N  
YIELD 71%

RX(10) RCT A 118-48-9, P 2617-79-0  
PRO N 24122-31-4  
CON 6 minutes, heated  
NTE a few drops of DMF used, green chemistry-solvent, microwave irradiation, no solvent

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 33 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 145:230582 CASREACT  
TITLE: Syntheses of 2-substituted  
6-bromomethyl-4(3H)-quinazolinones  
AUTHOR(S): Cao, Sheng-Li; Feng, Yu-Ping; Gao, Hong-He; Feng, Ke-Ran  
CORPORATE SOURCE: Department of Chemistry, Capital Normal University, Beijing, 100037, Peop. Rep. China  
SOURCE: Yingyong Huaxue (2005), 22(9), 1027-1029  
CODEN: YIHUED; ISSN: 1000-0518  
PUBLISHER: Kexue Chubanshe  
DOCUMENT TYPE: Journal  
LANGUAGE: Chinese  
GI



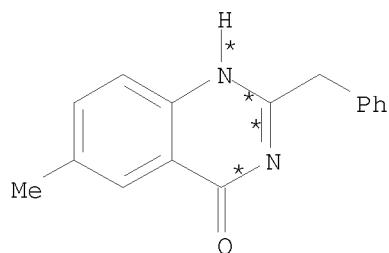
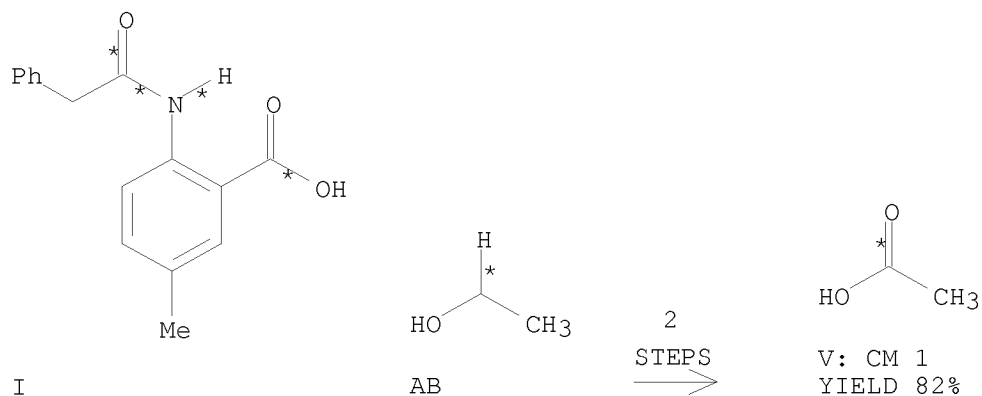
AB 2-Amino-5-methylbenzoic acid (I) was acylated with acyl chlorides, then heated with acetic anhydride to give 2-Ph or 2-benzyl-6-methylbenzoxazin-4-one, while I was reacted with propanoic anhydride or trifluoroacetic anhydride to give 2-Et or 2-trifluoromethyl-6-methyl-benzoxazin-4-one directly. Then, 2-substituted 6-methylbenzoxazin-4-ones were heated with formamide to afford 2-substituted 6-methyl-4(3H)-quinazolinones, which were converted into the title compds. II (R = Ph, CH<sub>2</sub>Ph, CH<sub>2</sub>CH<sub>3</sub>, CF<sub>3</sub>) via bromination with

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N-bromosuccinimide in the presence of (PhCOO)<sub>2</sub>. The structures of all the intermediates and final products were confirmed with ESI-MS, <sup>1</sup>H-NMR and elemental anal.

RX(18) OF 32 COMPOSED OF RX(4), RX(12)

RX(18) I + AB ==> V



V: CM 2  
YIELD 82%

RX(4) RCT I 157834-20-3  
RGT K 108-24-7 Ac2O  
PRO L 157834-12-3  
CON 3 hours, reflux

RX(12) RCT L 157834-12-3

STAGE(1)

RGT AC 75-12-7 Formamide  
CON 3 hours, 150 - 155 deg C

STAGE(2)

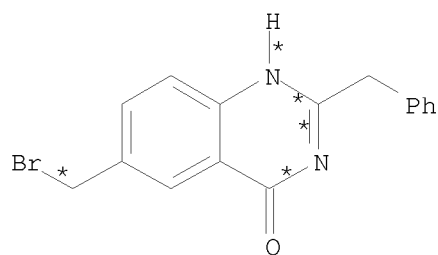
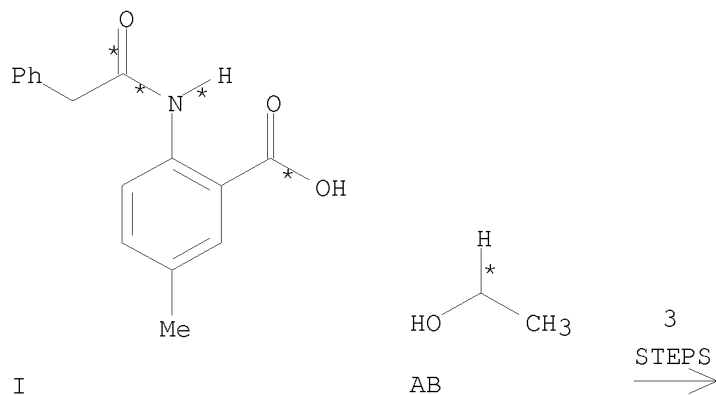
RCT AB 64-17-5  
SOL 7732-18-5 Water

PRO V 905455-25-6

RX(29) OF 32 COMPOSED OF RX(4), RX(12), RX(8)

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RX(29)      I   +   AB   ==>   W



W  
YIELD 44%

RX(4)      RCT   I 157834-20-3  
             RGT   K 108-24-7 Ac2O  
             PRO   L 157834-12-3  
             CON   3 hours, reflux

RX(12)     RCT   L 157834-12-3

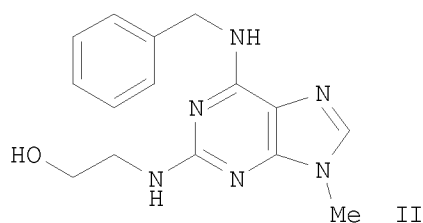
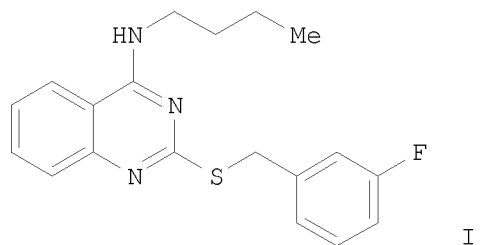
STAGE(1)  
      RGT   AC 75-12-7 Formamide  
      CON   3 hours, 150 - 155 deg C

STAGE(2)  
      RCT   AB 64-17-5  
      SOL   7732-18-5 Water

PRO   V 905455-25-6

RX(8)      RCT   V 905455-25-6  
             RGT   S 94-36-0 Benzoyl peroxide, T 128-08-5 Bromosuccinimide  
             PRO   W 905455-23-4  
             SOL   67-66-3 CHCl3  
             CON   3 hours, reflux

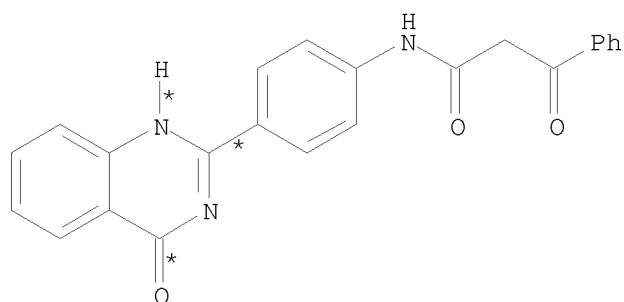
L3 ANSWER 34 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 145:124518 CASREACT  
 TITLE: An efficient direct amination of cyclic amides and cyclic ureas  
 AUTHOR(S): Wan, Zhao-Kui; Wacharasindhu, Sumrit; Binnun, Eva; Mansour, Tarek  
 CORPORATE SOURCE: Chemical and Screening Sciences, Wyeth Research, Cambridge, MA, 02140, USA  
 SOURCE: Organic Letters (2006), 8(11), 2425-2428  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



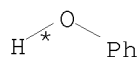
AB An efficient one-step amination of cyclic amides and ureas has been developed. Treatment of cyclic amides and cyclic ureas with BOP in the presence of DBU in various solvents led to the formation of cyclic amidines and cyclic guanidines, e.g., I, in good to excellent yields. Concise syntheses of biol. intriguing kinetin and potent kinase inhibitor olomoucine (II) were thus achieved in just one and two steps, resp.

RX(21) OF 40 AB + AS ==> AT

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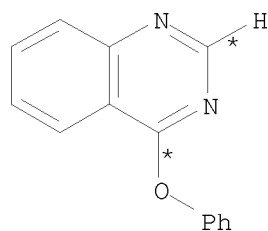


AB



AS

(21)  $\longrightarrow$



AT

YIELD 84%

RX(21) RCT AB 95812-45-6

STAGE(1)

RGT D 6674-22-2 DBU, E 56602-33-6 BOP reagent, F 101-84-8 PhOPh

SOL 75-05-8 MeCN

CON 5 - 10 minutes, room temperature

STAGE(2)

RCT AS 108-95-2

CON 10 hours, room temperature

PRO AT 16347-97-0

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 35 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 145:47552 CASREACT

TITLE: Chemical Development of ZD9331: Synthesis of a Bromomethylquinazolinone Avoiding a Nonselective Radical Bromination

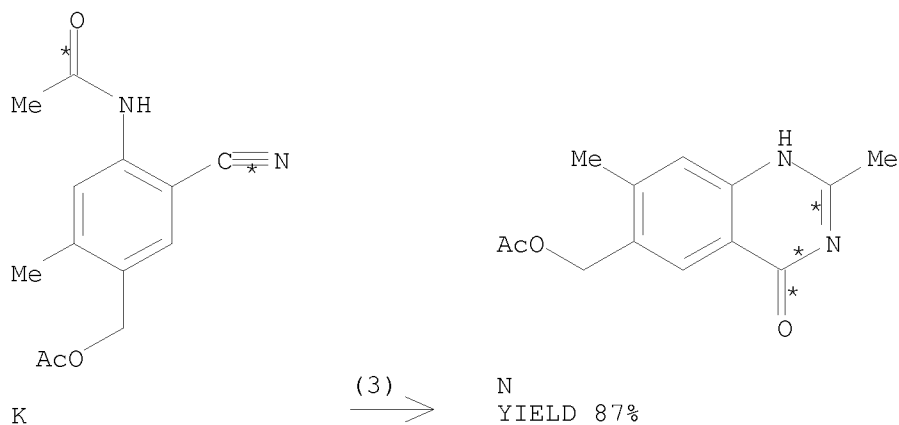
AUTHOR(S): Bentley, Dagmar; Godfrey, Andrew A.; Warren, Kenneth E. H.

CORPORATE SOURCE: Process Research and Development Department, AstraZeneca, Macclesfield, Cheshire, SK10 2NA, UK

SOURCE: Organic Process Research & Development (2006), 10(3), 553-555  
 CODEN: OPRDFK; ISSN: 1083-6160  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB An efficient regiospecific synthesis of ZD9331 Pivaloyloxymethyl (POM) Bromide has been accomplished via ZD9331 Quinacetate HCl avoiding a nonselective bromination. The original route used a radical bromination on a substrate with three Me groups, which generated a range of bromomethyl derived compds. that carried through to the final active pharmaceutical ingredient (API). A strategy, based on the Zinin reaction, was developed to synthesize the required bromomethyl compound in a regioselective manner. This approach was successfully scaled to manufacture a ton of material.

RX(3) OF 6 ...K ==> N



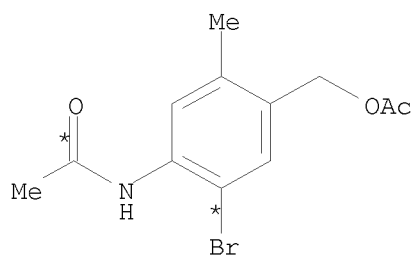
RX(3) RCT K 838858-87-0  
 RGT O 7647-01-0 HCl  
 PRO N 838858-86-9  
 SOL 57-55-6 MeCHOHCH2OH  
 CON SUBSTAGE(1) 60 minutes, room temperature  
 SUBSTAGE(2) 30 deg C  
 NTE HCl gas used

RX(5) OF 6 COMPOSED OF RX(2), RX(3)

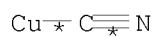
RX(5) B + D ==> N



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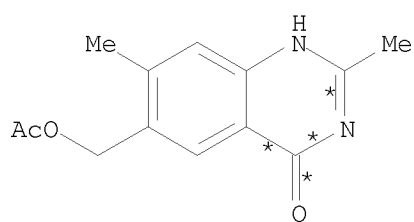


B



D

2  
STEPS  
→



N

YIELD 87%

RX(2) RCT B 838858-88-1, D 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT L 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

SUBSTAGE(3) 90 deg C -> 50 deg C

PRO K 838858-87-0

RX(3)

RCT K 838858-87-0

RGT O 7647-01-0 HCl

PRO N 838858-86-9

SOL 57-55-6 MeCHOHCH<sub>2</sub>OH

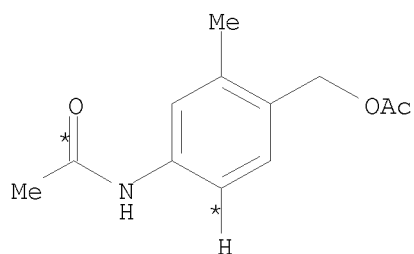
CON SUBSTAGE(1) 60 minutes, room temperature

SUBSTAGE(2) 30 deg C

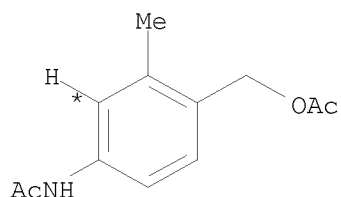
NTE HCl gas used

RX(6) OF 6 COMPOSED OF RX(1), RX(2), RX(3)

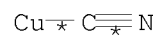
RX(6) 2 A + D ==> N



A

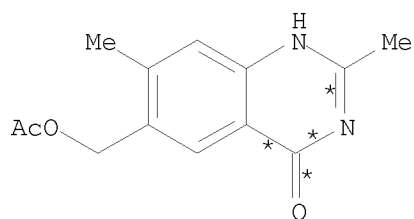


A



D

3  
STEPS  
→



N  
YIELD 87%

RX(1)

STAGE(1)

RGT D 544-92-3 CuCN, E 121-44-8 Et3N, F 75-36-5 AcCl

SOL 141-78-6 AcOEt

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -&gt; 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 30 minutes, 50 deg C

SUBSTAGE(5) 50 deg C -&gt; 20 deg C

STAGE(2)

RCT A 890086-36-9

RGT G 77-48-5 Br2-Me2-hydantoin

SOL 75-05-8 MeCN

CON SUBSTAGE(1) 60 minutes, 50 deg C

SUBSTAGE(2) 50 deg C -&gt; 20 deg C

STAGE(3)

RGT H 7732-18-5 Water

PRO B 838858-88-1, C 890086-37-0

NTE regioselective

RX(2)

RCT B 838858-88-1, D 544-92-3

## STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -&gt; 60 deg C

## STAGE(2)

RGT L 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -&gt; 90 deg C

SUBSTAGE(3) 90 deg C -&gt; 50 deg C

PRO K 838858-87-0

## RX(3)

RCT K 838858-87-0

RGT O 7647-01-0 HCl

PRO N 838858-86-9

SOL 57-55-6 MeCHOHCH2OH

CON SUBSTAGE(1) 60 minutes, room temperature

SUBSTAGE(2) 30 deg C

NTE HCl gas used

## REFERENCE COUNT:

10

THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 36 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 144:432671 CASREACT

TITLE: Synthesis and structure of  
4-amino-1,2-dihydro-2-oxo-3-quinolinecarboxylate  
estersAUTHOR(S): Ukrainets, I. V.; Bezugly, P. O.; Nicola, Skaif;  
Gorokhova, O. V.; Sidorenko, L. V.

CORPORATE SOURCE: Nats. Farm. Univ., Kharkov, 61002, Ukraine

SOURCE: Zhurnal Organichnoi ta Farmatsevtichnoi Khimii (2004),  
2(2), 56-61

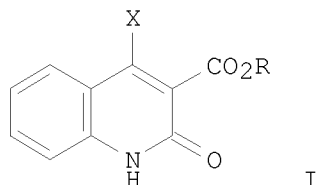
CODEN: ZOFKAM

PUBLISHER: Natsional'nii Farmatsevtichnii Universitet

DOCUMENT TYPE: Journal

LANGUAGE: Russian

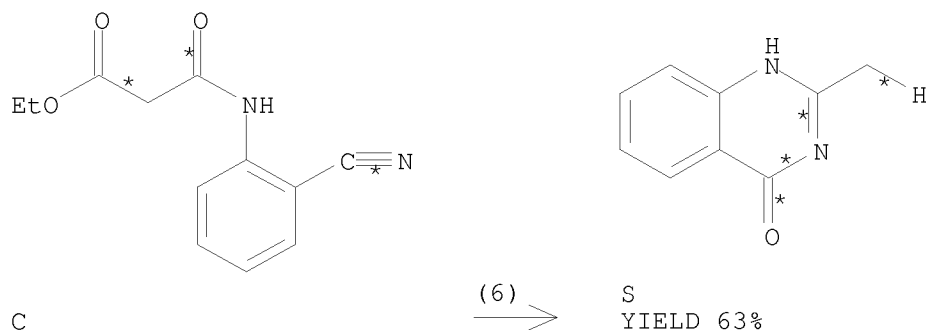
GI



AB Title compds. I (R = Me, Et; X = NH<sub>2</sub>) were prepared by heterocyclization of 2-NCC6H<sub>4</sub>NHCOCH<sub>2</sub>COOEt in R<sub>2</sub>Na/ROH. I (R = Et, X = NH<sub>2</sub>) was also prepared from I (R = Et, X = Cl) via a pyridinium salt. I (R = Me, X = NH<sub>2</sub>) was subjected to x-ray anal.

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RX(6) OF 26 ...C ==> S



RX(6) RCT C 130427-06-4

STAGE(1)

RGT R 1310-58-3 KOH  
SOL 7732-18-5 Water  
CON 5 hours, reflux

STAGE(2)

RGT G 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON pH 4

PRO S 1769-24-0

NTE alternative preparation shown, product depends on temperature

L3 ANSWER 37 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 144:370022 CASREACT

TITLE: Studies on quinazolines, 12. Design of  
4-amino-8-arylquinazoline derivatives as potential  
non-peptide corticotropin-releasing hormone receptor I  
(CRHR1) antagonists

AUTHOR(S): Wu, Fe-lin Lin; Chen, Grace Shiahuy; Chen, Mei-Yu;  
Cheng, Fong-Chi; Chern, Ji-Wang

CORPORATE SOURCE: School of Pharmacy, College of Medicine, National  
Taiwan University, Taichung, Taiwan

SOURCE: Chinese Pharmaceutical Journal (Taipei, Taiwan)  
(2004), 56(2), 97-109

CODEN: CPHJEP; ISSN: 1016-1015

PUBLISHER: Pharmaceutical Society of Republic of China

DOCUMENT TYPE: Journal

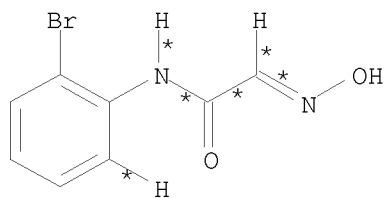
LANGUAGE: English

AB Four 8-aryl-4-(N-cyclopropylmethyl-N-propyl)amino-2-methylquinazolines  
were synthesized, and their binding affinity for corticotropin-releasing  
hormone type 1 receptor (CRHR1) was investigated. Two of the compds.  
possessed high rCRHR1 affinities of  $K_i = 13$  and  $50$  nM. The quinazoline  
derivs. showed comparable SAR to the other known bicyclic system; the  
ortho-substituent on the 8-aryl ring is indispensable.

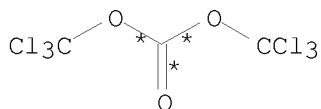
10/ 562,112

RX(52) OF 92 COMPOSED OF RX(2), RX(3), RX(4), RX(5), RX(6)

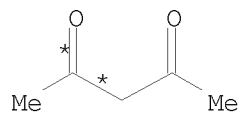
RX(52) C + L + R ==> S



C

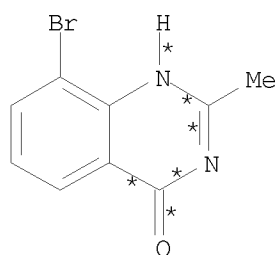


L



R

5  
STEPS  
→



S

YIELD 51%

RX(2) RCT C 101080-38-0  
RGT E 7664-93-9 H2SO4  
PRO H 20780-74-9  
CON 30 minutes, 85 - 87 deg C

RX(3) RCT H 20780-74-9

STAGE(1)

RGT J 1310-73-2 NaOH, K 7722-84-1 H2O2  
SOL 7732-18-5 Water  
CON 0 deg C

STAGE(2)

RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON pH 4

PRO I 20776-51-6

RX(4) RCT I 20776-51-6, L 32315-10-9  
PRO M 331646-98-1  
SOL 109-99-9 THF  
CON 2 hours, reflux

RX(5) RCT M 331646-98-1  
RGT P 1336-21-6 NH4OH, Q 631-61-8 NH4OAc  
PRO O 437998-34-0  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 60 deg C -> 95 deg C

SUBSTAGE(2) 1 hour, 95 deg C

RX(6) RCT O 437998-34-0, R 123-54-6  
 PRO S 221298-74-4  
 CAT 104-15-4 TsOH  
 SOL 75-05-8 MeCN  
 CON 3 hours, reflux  
 NTE alternative solvent/THF shown

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 38 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 144:292686 CASREACT

TITLE: Multi-component synthesis of 3,2-substituted  
 quinazolin-4(3H)-ones under solvent-free conditions

AUTHOR(S): Dandia, Anshu; Singh, Ruby; Sarawgi, Pritima

CORPORATE SOURCE: Department of Chemistry, University of Rajasthan,  
 Jaipur, 302004, India

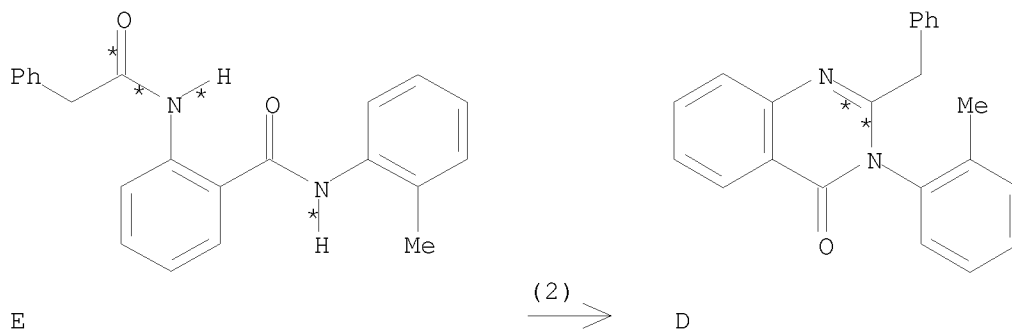
SOURCE: International Electronic Conferences on Synthetic  
 Organic Chemistry, 5th, 6th, Sept. 1-30, 2001 and 2002  
 [and] 7th, 8th, Nov. 1-30, 2003 and 2004 (2004),  
 1116-1122. Editor(s): Seijas, Julio A. Molecular  
 Diversity Preservation International: Basel, Switz.  
 CODEN: 69GTCO

DOCUMENT TYPE: Conference; (computer optical disk)

LANGUAGE: English

AB Rapid one-pot solvent-free procedure has been developed for the synthesis  
 of 2,3-disubstituted quinazolin-4(3H)-ones by neat three component  
 cyclocondensation of anthranilic acid, Ph acetyl chloride/benzoyl chloride  
 and substituted anilines under microwave irradiation The exptl. methodol. and  
 microwave conditions described here are well established, allowing  
 significant rate enhancement and good yields compared to multistep  
 conventional reaction conditions. The reaction is generalized for o, m &  
 p substituted anilines with electron donating and withdrawing groups to  
 give quinazolin-4(3H)-ones. Ortho substituted anilines fail to undergo  
 ring closure quinazolines under conventional conditions. The detailed  
 reaction mechanism of title reaction has also been discussed.

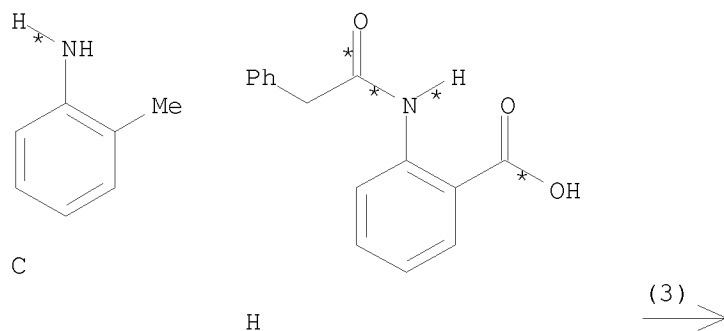
RX(2) OF 22 ...E ==> D



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RX(2)      RCT   E 879126-67-7  
             PRO   D 19857-39-7  
             CAT   104-15-4 TsOH  
             SOL   68-12-2 DMF  
             NTE   microwave irradi., alternative preparation shown

RX(3) OF 22      C + H ==> D

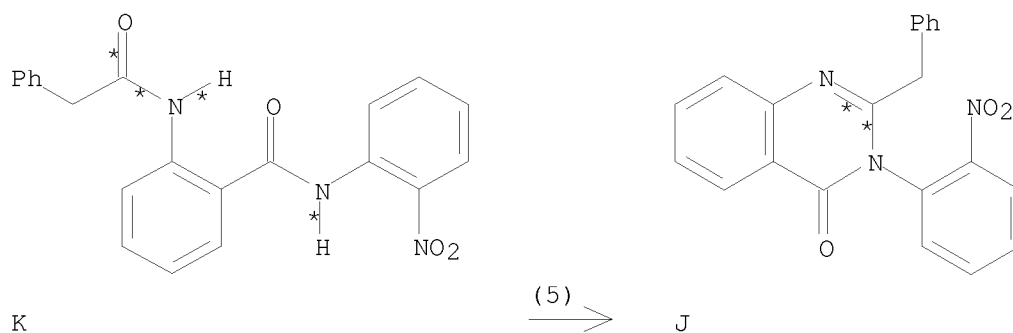


D  
YIELD 91%

RX(3)      RCT   C 95-53-4, H 28565-98-2  
             PRO   D 19857-39-7  
             CON   4 minutes  
             NTE   microwave irradi., 640 W used, alternative preparation shown

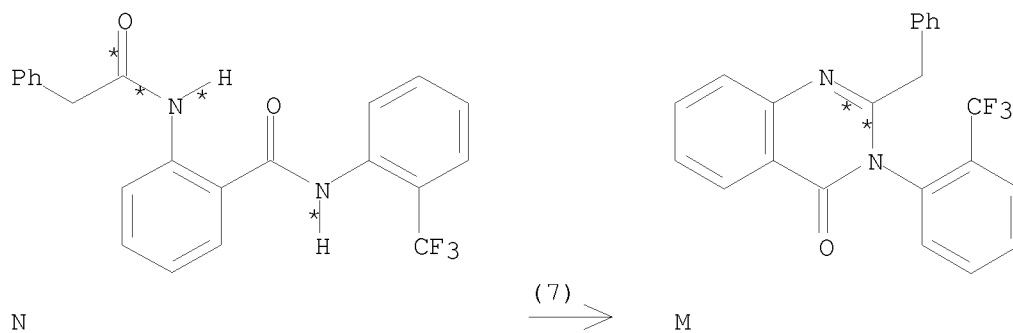
RX(5) OF 22      ...K ==> J

10/ 562,112



RX(5)      RCT   K 879126-68-8  
             PRO   J 201293-03-0  
             CAT   104-15-4 TsOH  
             SOL   68-12-2 DMF  
             NTE   microwave irradi., alternative preparation shown

RX(7) OF 22      ...N ==> M

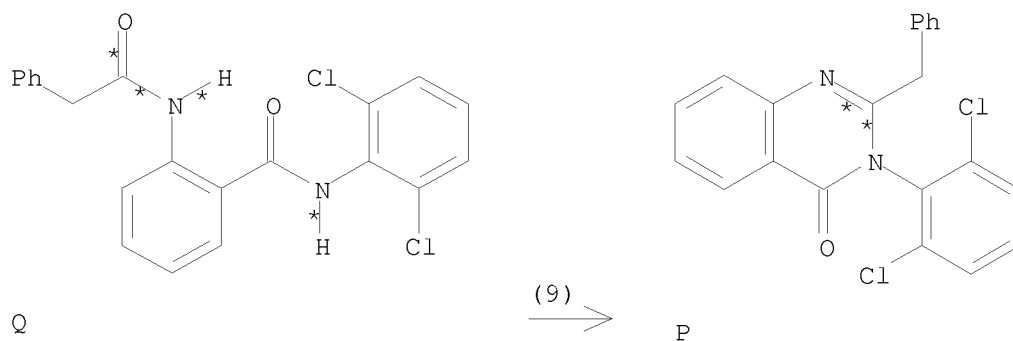


RX(7)      RCT   N 848085-17-6  
             PRO   M 848085-22-3  
             CAT   104-15-4 TsOH  
             SOL   68-12-2 DMF  
             NTE   microwave irradi., alternative preparation shown

RX(9) OF 22      ...Q ==> P

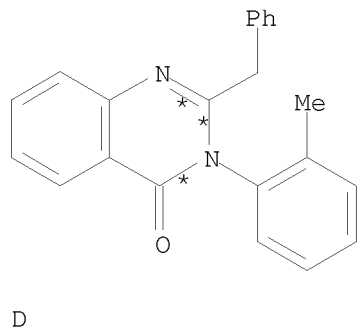
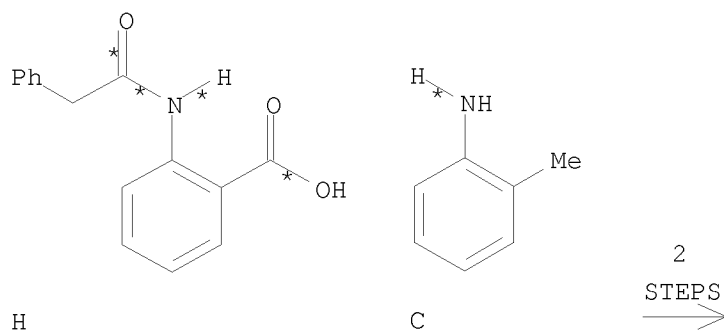


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RX(9) RCT Q 824972-68-1  
 PRO P 381194-40-7  
 CAT 104-15-4 TsOH  
 SOL 68-12-2 DMF  
 NTE microwave irradiation, alternative preparation shown

RX(19) OF 22 COMPOSED OF RX(15), RX(2)  
 RX(19) H + C ==> D



RX(15) RCT H 28565-98-2  
 STAGE(1)

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RGT AB 1318-93-0 Montmorillonite, AC 108-24-7 Ac2O

STAGE(2)

RCT C 95-53-4

PRO E 879126-67-7

NTE chemoselective, green chem., microwave irradi., Montmorillonite  
KSF used

RX(2) RCT E 879126-67-7

PRO D 19857-39-7

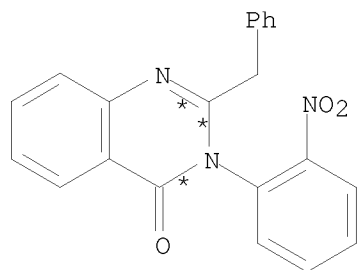
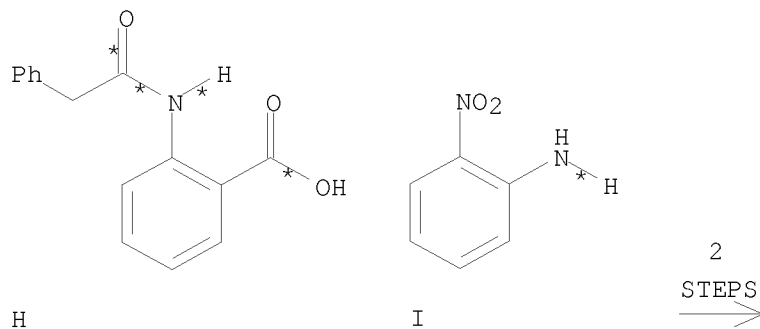
CAT 104-15-4 TsOH

SOL 68-12-2 DMF

NTE microwave irradi., alternative preparation shown

RX(20) OF 22 COMPOSED OF RX(16), RX(5)

RX(20) H + I ==> J



J

RX(16) RCT H 28565-98-2

STAGE(1)

RGT AB 1318-93-0 Montmorillonite, AC 108-24-7 Ac2O

STAGE(2)

RCT I 88-74-4

PRO K 879126-68-8

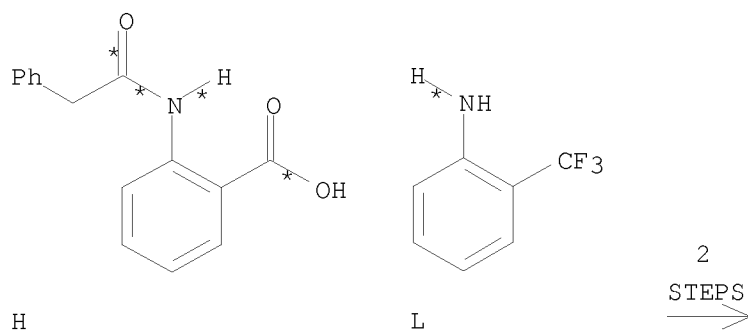
NTE chemoselective, green chem., microwave irradi., Montmorillonite

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KSF used

RX(5) RCT K 879126-68-8  
PRO J 201293-03-0  
CAT 104-15-4 TsOH  
SOL 68-12-2 DMF  
NTE microwave irradiation, alternative preparation shown

RX(21) OF 22 COMPOSED OF RX(17), RX(7)  
RX(21) H + L ==> M



M

RX(17) RCT H 28565-98-2

STAGE(1)

RGT AB 1318-93-0 Montmorillonite, AC 108-24-7 Ac2O

STAGE(2)

RCT L 88-17-5

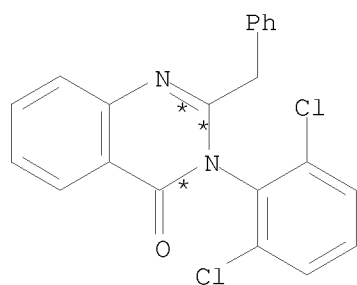
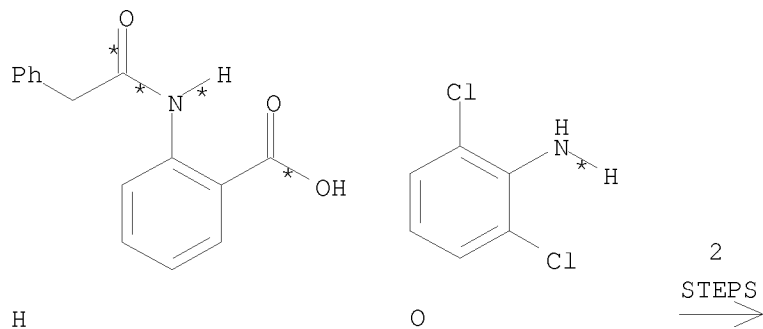
PRO N 848085-17-6

NTE chemoselective, green chem., microwave irradiation, Montmorillonite  
KSF used

RX(7) RCT N 848085-17-6  
PRO M 848085-22-3  
CAT 104-15-4 TsOH  
SOL 68-12-2 DMF  
NTE microwave irradiation, alternative preparation shown

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RX(22) OF 22 COMPOSED OF RX(18), RX(9)  
RX(22) H + O ==> P



P

RX(18) RCT H 28565-98-2

STAGE(1)

RGT AB 1318-93-0 Montmorillonite, AC 108-24-7 Ac2O

STAGE(2)

RCT O 608-31-1

PRO Q 824972-68-1

NTE chemoselective, green chem., microwave irradiation, Montmorillonite KSF used

RX(9) RCT Q 824972-68-1

PRO P 381194-40-7

CAT 104-15-4 TsOH

SOL 68-12-2 DMF

NTE microwave irradiation, alternative preparation shown

REFERENCE COUNT:

29

THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 39 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 144:205151 CASREACT

TITLE: Discovery of potent and selective PARP-1 and PARP-2 inhibitors: SBDD analysis via a combination of X-ray structural study and homology modeling

AUTHOR(S): Ishida, Junya; Yamamoto, Hirofumi; Kido, Yoshiyuki; Kamiyo, Kazunori; Murano, Kenji; Miyake, Hiroshi; Ohkubo, Mitsuru; Kinoshita, Takayoshi; Warizaya, Masaichi; Iwashita, Akinori; Mihara, Kayoko; Matsuoka, Nobuya; Hattori, Kouji

CORPORATE SOURCE: Medicinal Chemistry Research Laboratories, Fujisawa Pharmaceutical Co. Ltd, 5-2-3 Tokodai, Tsukuba, Ibaraki, 300-2698, Japan

SOURCE: Bioorganic &amp; Medicinal Chemistry (2006), 14(5), 1378-1390

CODEN: BMECEP; ISSN: 0968-0896

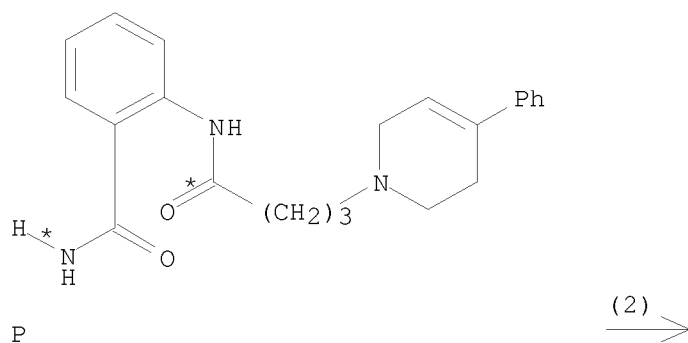
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

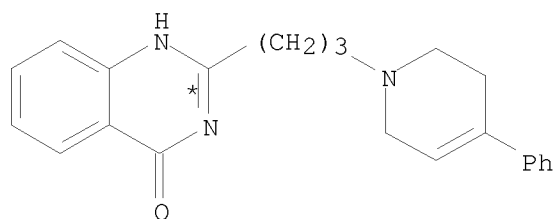
LANGUAGE: English

AB We disclose herein our efforts aimed at discovery of selective PARP-1 and PARP-2 inhibitors. We have recently discovered several novel classes of quinazolinones, quinazolidinones, and quinoxalines as potent PARP-1 inhibitors, which may represent attractive therapeutic candidates. In PARP enzyme assays using recombinant PARP-1 and PARP-2, the quinazolinone derivs. displayed relatively high selectivity for PARP-1 and quinoxaline derivs. showed superior selectivity for PARP-2, and the quinazolidinone derivs. did not have selectivity for PARP-1/2. Structure-based drug design anal. via a combination of X-ray structural study utilizing the complexes of inhibitors and human PARP-1 catalytic domain, and homol. modeling using murine PARP-2 suggested distinct interactions of inhibitors with PARP-1 and PARP-2. These findings provide a new structural framework for the design of selective inhibitors for PARP-1 and PARP-2.

RX(2) OF 47 ...P ==&gt; D



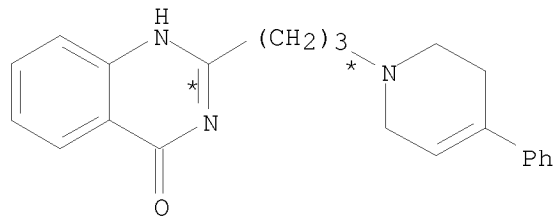
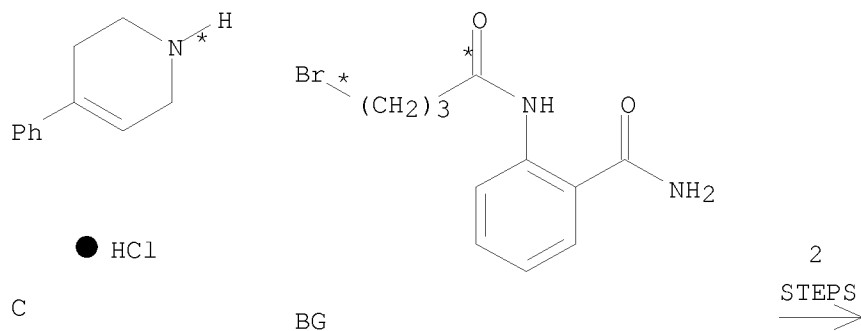
10/ 562,112



D  
YIELD 74%

RX(2) RCT P 437998-41-9  
RGT J 1310-73-2 NaOH  
PRO D 437995-37-4  
SOL 7732-18-5 Water, 123-91-1 Dioxane  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 15 hours, room temperature

RX(35) OF 47 COMPOSED OF RX(26), RX(2)  
RX(35) C + BG ==> D



D  
YIELD 74%

RX(26) RCT C 43064-12-6, BG 437998-35-1  
STAGE(1)  
RGT T 121-44-8 Et3N

SOL 68-12-2 DMF  
 CON SUBSTAGE(1) 0 deg C  
 SUBSTAGE(2) 0 deg C -> room temperature  
 SUBSTAGE(3) 24 hours, room temperature

STAGE(2)  
 RGT N 7732-18-5 Water  
 CON room temperature

PRO P 437998-41-9

RX(2) RCT P 437998-41-9  
 RGT J 1310-73-2 NaOH  
 PRO D 437995-37-4  
 SOL 7732-18-5 Water, 123-91-1 Dioxane  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 15 hours, room temperature

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 40 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 144:192275 CASREACT

TITLE: Preparation of quinazolinone derivatives useful for  
 the regulation of glucose homeostasis and food intake

INVENTOR(S): Rudolph, Joachim; O'Connor, Stephen; Coish, Philip;  
 Wickens, Philip; Bondar, Georgiy; Chuang, Chih-Yuan;  
 Ramsden, Philip; Lowe, Derek; Bierer, Donald; Chen,  
 Libing; Fu, Wenlang; Khire, Uday; Liu, Xiao-Gao;  
 McClure, Andrea; Wang, Lei; Yi, Lin; Esler, William

PATENT ASSIGNEE(S): Bayer Pharmaceuticals Corporation, USA

SOURCE: PCT Int. Appl., 559 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006012577	A2	20060202	WO 2005-US26192	20050722
WO 2006012577	A3	20060928		

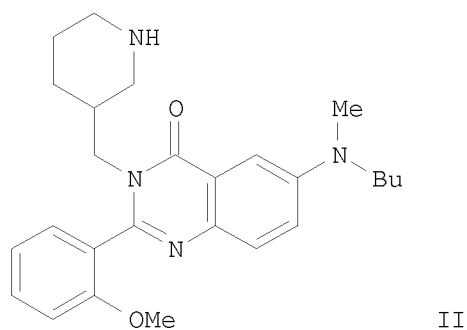
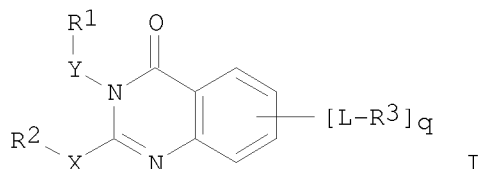
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,  
 CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,  
 GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,  
 LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,  
 NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,  
 SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,  
 ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,  
 IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,  
 CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,  
 GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,  
 KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-590804P 20040722

OTHER SOURCE(S): MARPAT 144:192275

GI

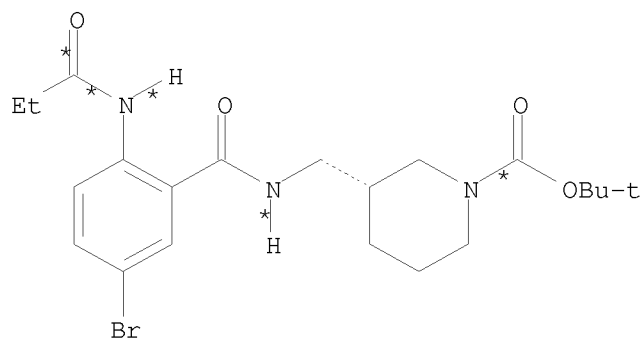


AB The invention is related to substituted quinazolinone derivs. I [R1 = (un)substituted pyrrolidin-3-yl, piperidin-3-yl, morpholin-4-yl, etc.; R2 = H, (un)substituted cyclo/alkyl, pyridinyl, Ph, etc.; R3 = H, halo, haloalkyl, (un)substituted Ph, alkyl, etc.; L = a bond, O, CO, S, SO2, NHSO2, NH and derivs., etc.; X = (CH2)m; m = 0-2; Y = (CH2)n; n = 1-2; p = 0-2; with provisos], and their pharmaceutically acceptable salts, and their compns., and methods for treating diabetes, obesity and related disorders, and regulation of glucose homeostasis and food intake (e.g., stimulation and suppression) (no data). The invention is also related to the preparation of quinazolinones I. Five biol. tests are given (no data). Thus, II•TFA was prepared by amination of 5-fluoro-2-nitrobenzoic acid with N-methylbutylamine, reduction of the nitro compound, cyclocondensation with o-anisoyl chloride, reaction with tert-Bu 3-(aminomethyl)piperidine-1-carboxylate (intermediate not isolated), and Boc-deprotection in the presence of TFA.

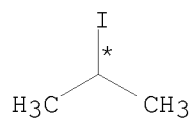
RX(128) OF 652 KL + Z ==> BH...



10/ 562,112

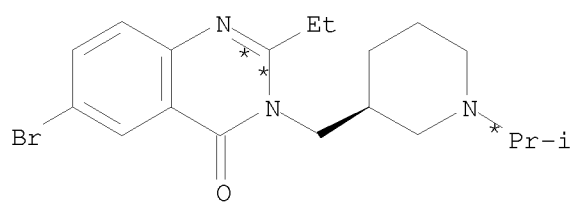


KL



Z

(128)  
→



BH

RX(128) RCT KL 875269-77-5

STAGE(1)

SOL 64-19-7 AcOH

CON 2 hours, 100 deg C

STAGE(2)

RCT Z 75-30-9

RGT AB 584-08-7 K<sub>2</sub>CO<sub>3</sub>

SOL 75-05-8 MeCN

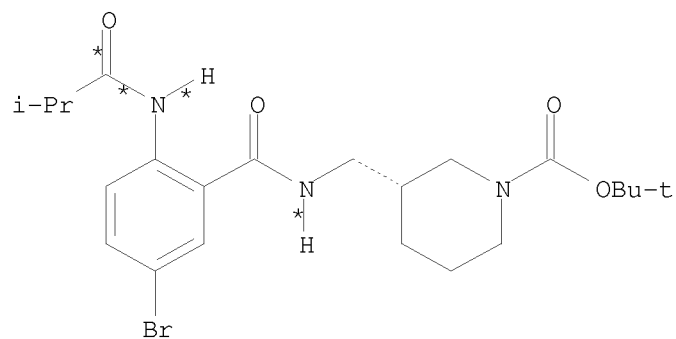
CON 4 hours, 70 deg C

PRO BH 875269-76-4

NTE sealed vial used in stage 1

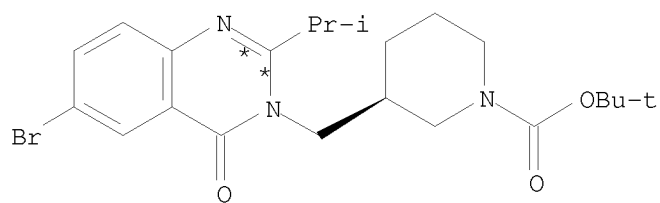
RX(137) OF 652 ...KT ==> KS...

10/ 562,112



KT

(137)  
→

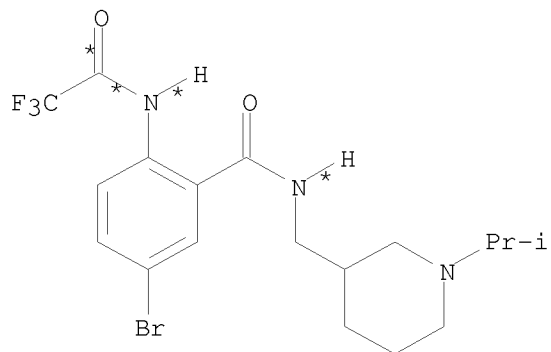


KS

YIELD 38%

RX(137)    RCT    KT 875269-98-0  
             RGT    EB 1310-65-2 LiOH  
             PRO    KS 875269-86-6  
             SOL    107-21-1 (CH<sub>2</sub>OH)<sub>2</sub>  
             CON    15 hours, 130 deg C

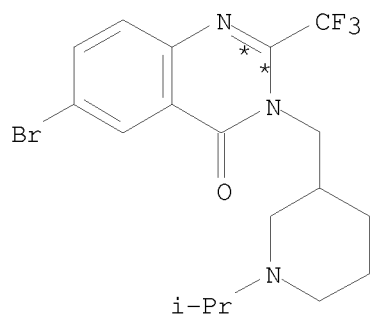
RX(162) OF 652    ...LQ ==> FL...



LQ

(162)  
→

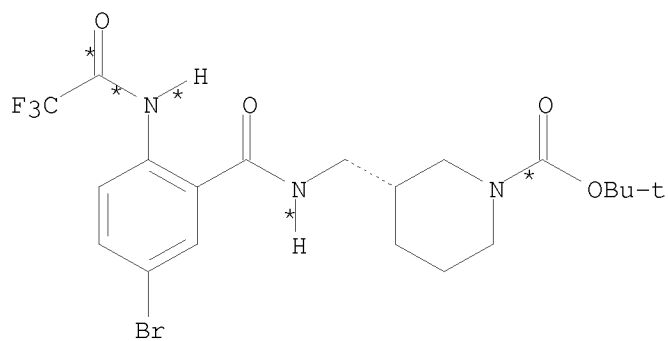
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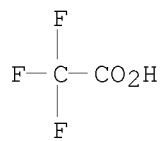
FL  
YIELD 95%

RX(162)    RCT    LQ 875270-14-7  
             PRO    FL 875270-15-8  
             CON    1 hour, 200 deg C  
             NTE    thermal, sealed vial used

RX(164) OF 652    ...LR + C ==> LS...

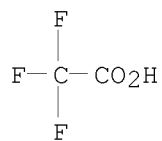


LR

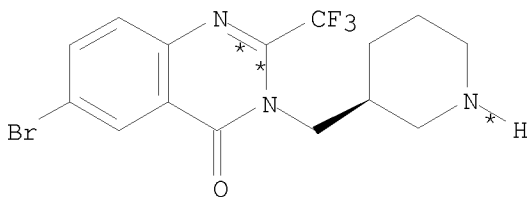


C

(164)  
→



LS: CM 1  
YIELD 100%



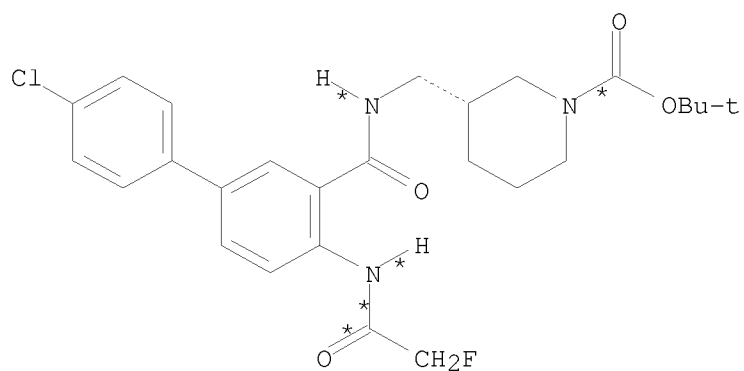
LS: CM 2  
YIELD 100%

RX(164)    RCT    LR 875270-16-9, C 76-05-1  
             PRO    LS 875270-18-1

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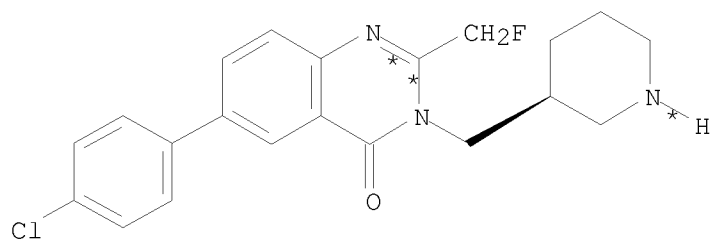
CON 1 hour, 150 deg C  
NTE microwave irradiation

RX(169) OF 652 ...LX ==&gt; GC...



LX

(169)

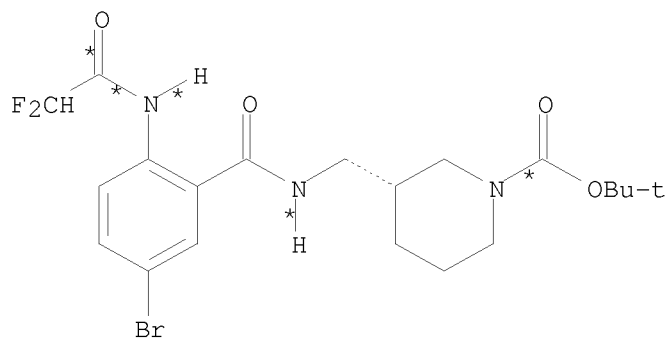


GC  
YIELD 87%

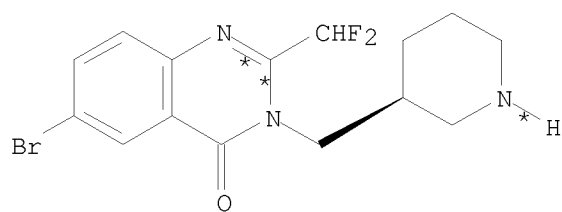
RX(169)	RCT	LX 875270-26-1
	RGT	LY 109-63-7 BF3-Et2O
	PRO	GC 875270-27-2
	SOL	64-19-7 AcOH
	CON	25 minutes, 130 deg C
	NTE	microwave irradiation

RX(171) OF 652 ...MA ==&gt; MD...

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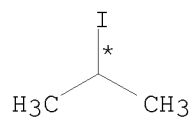
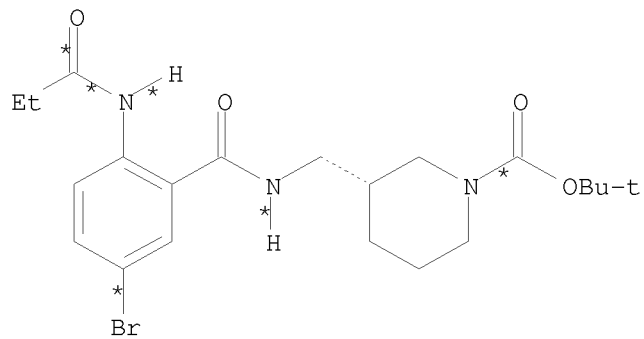


(171)  
→

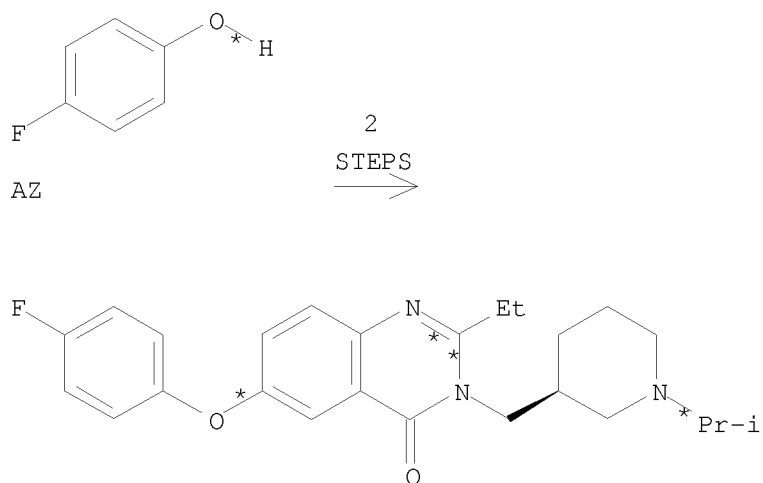


RX(171)    RCT    MA 875270-28-3  
             PRO    MD 875270-29-4  
             SOL    64-19-7 AcOH  
             CON    2 hours, 100 deg C  
             NTE    sealed vial used

RX(264) OF 652 COMPOSED OF RX(128), RX(19)  
RX(264)    KL   +   Z   +   AZ   ==>   BI



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BI

RX(128) RCT KL 875269-77-5

STAGE(1)

SOL 64-19-7 AcOH

CON 2 hours, 100 deg C

STAGE(2)

RCT Z 75-30-9

RGT AB 584-08-7 K<sub>2</sub>CO<sub>3</sub>

SOL 75-05-8 MeCN

CON 4 hours, 70 deg C

PRO BH 875269-76-4

NTE sealed vial used in stage 1

RX(19) RCT AZ 371-41-5, BH 875269-76-4

RGT BC 1118-71-4 3,5-Heptanedione, 2,2,6,6-tetramethyl-, AH 534-17-8  
Cs<sub>2</sub>CO<sub>3</sub>

PRO BI 875258-87-0

CAT 7758-89-6 CuCl

SOL 872-50-4 NMEP

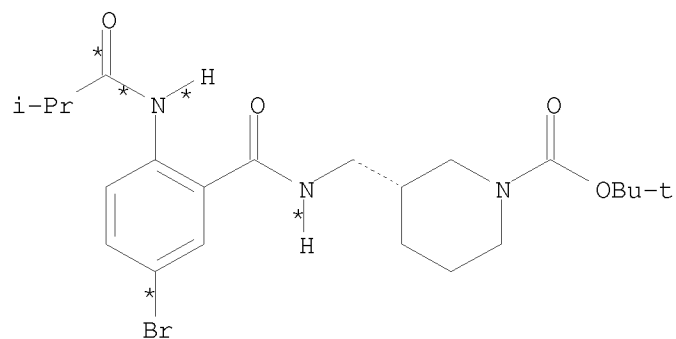
CON 20 minutes, room temperature -> 205 deg C

NTE thermal, microwave irradiation, sealed tube used, Ullmann  
coupling reaction

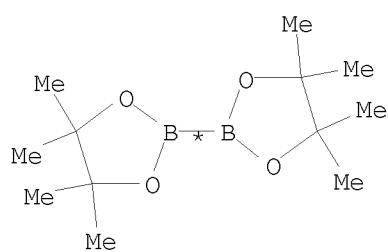
RX(285) OF 652 COMPOSED OF RX(137), RX(138)

RX(285) KT + KU ==> KV

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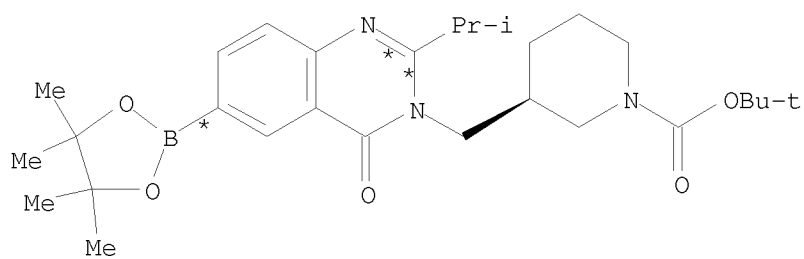


KT



KU

2  
STEPS  
→



KV

YIELD 82%

RX(137)    RCT    KT 875269-98-0  
              RGT    EB 1310-65-2 LiOH  
              PRO    KS 875269-86-6  
              SOL    107-21-1 (CH<sub>2</sub>OH)<sub>2</sub>  
              CON    15 hours, 130 deg C

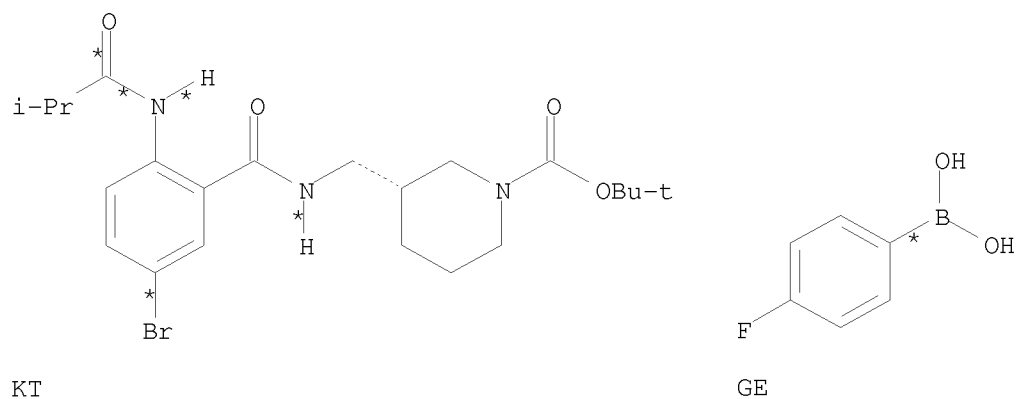
RX(138)    RCT    KS 875269-86-6, KU 73183-34-3  
              RGT    KW 127-08-2 AcOK  
              PRO    KV 875269-87-7  
              CAT    72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-  
                  κP)ferrocene]dichloro-, (SP-4-2)-  
              SOL    68-12-2 DMF

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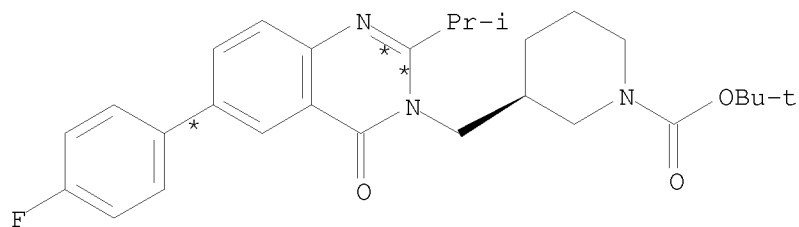
CON SUBSTAGE(1) 2 minutes, room temperature  
SUBSTAGE(2) 15 hours, room temperature -> 60 deg C  
SUBSTAGE(3) 60 deg C -> room temperature  
NTE Suzuki coupling reaction

RX(286) OF 652 COMPOSED OF RX(137), RX(151)

RX(286) KT + GE ==> DT



2  
STEPS  
→



YIELD 94%

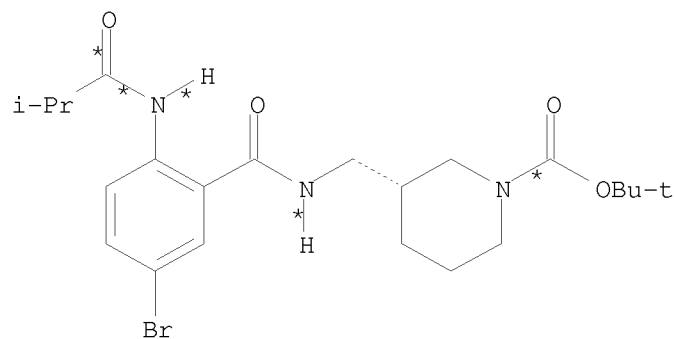
RX(137) RCT KT 875269-98-0  
RGT EB 1310-65-2 LiOH  
PRO KS 875269-86-6  
SOL 107-21-1 (CH2OH)2  
CON 15 hours, 130 deg C

RX(151) RCT KS 875269-86-6, GE 1765-93-1  
RGT AB 584-08-7 K2CO3  
PRO DT 875269-99-1  
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-  
SOL 7732-18-5 Water, 123-91-1 Dioxane, 108-88-3 PhMe  
CON 15 hours, 80 deg C  
NTE Suzuki coupling reaction

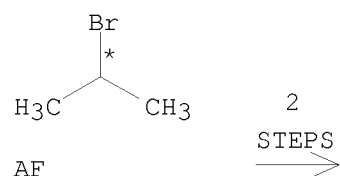


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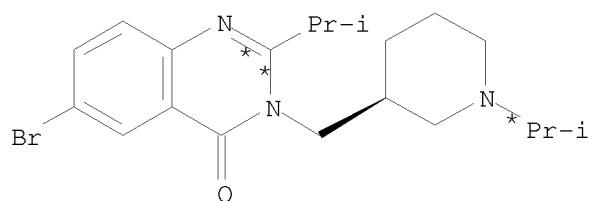
RX(287) OF 652 COMPOSED OF RX(137), RX(157)  
RX(287) KT + AF ==> ET



KT



AF



ET

RX(137) RCT KT 875269-98-0  
RGT EB 1310-65-2 LiOH  
PRO KS 875269-86-6  
SOL 107-21-1 (CH2OH)2  
CON 15 hours, 130 deg C

RX(157) RCT KS 875269-86-6

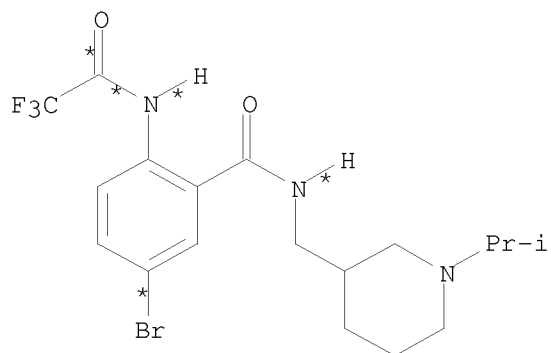
STAGE(1)  
RGT C 76-05-1 F3CCO2H  
SOL 75-09-2 CH2Cl2  
CON 3 hours, room temperature

STAGE(2)  
RCT AF 75-26-3  
RGT AH 534-17-8 Cs2CO3  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) 14 hours, 70 deg C  
SUBSTAGE(2) 70 deg C -> room temperature

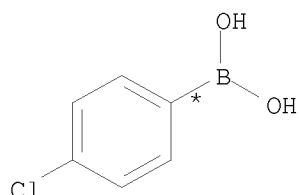
PRO ET 875270-09-0

RX(318) OF 652 COMPOSED OF RX(162), RX(57)  
RX(318) LQ + EV ==> FM

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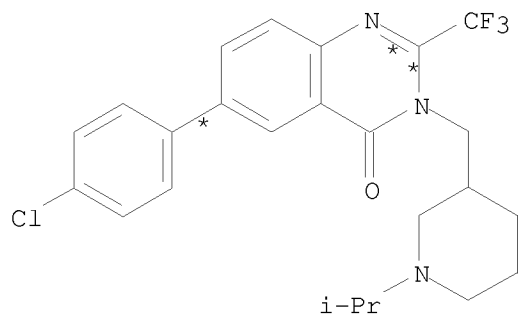


LQ



EV

2  
STEPS  
→



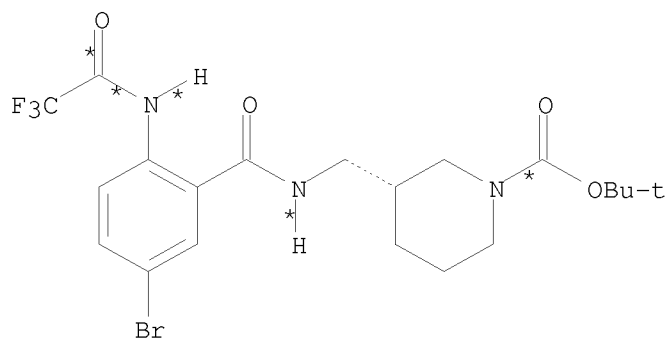
FM  
YIELD 14%

RX(162) RCT LQ 875270-14-7  
PRO FL 875270-15-8  
CON 1 hour, 200 deg C  
NTE thermal, sealed vial used

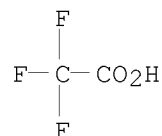
RX(57) RCT EV 1679-18-1, FL 875270-15-8  
RGT AB 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO FM 875259-36-2  
CAT 95464-05-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-, compd. with dichloromethane (1:1)  
SOL 109-99-9 THF  
CON 20 minutes, room temperature → 150 deg C  
NTE thermal, microwave irradiation, Suzuki coupling reaction, sealed tube used

RX(320) OF 652 COMPOSED OF RX(164), RX(165)  
RX(320) LR + C + Z ==> FN

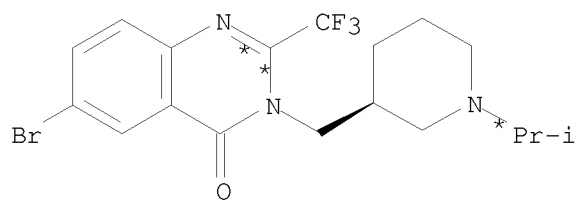
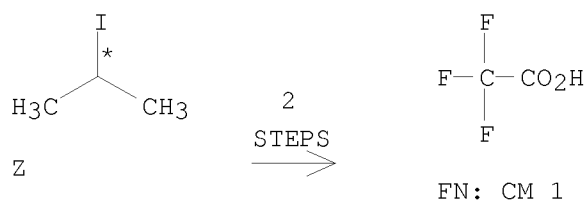
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LR



C



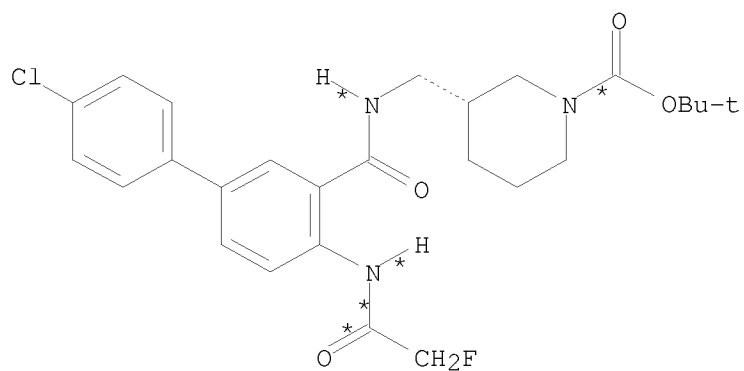
FN: CM 2

RX(164) RCT LR 875270-16-9, C 76-05-1  
PRO LS 875270-18-1  
CON 1 hour, 150 deg C  
NTE microwave irradiation

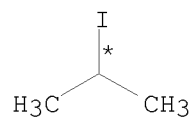
RX(165) RCT Z 75-30-9, LS 875270-18-1  
RGT AB 584-08-7 K2CO3  
PRO FN 875270-20-5  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 15 hours, room temperature -> 70 deg C  
SUBSTAGE(3) 70 deg C -> room temperature

RX(325) OF 652 COMPOSED OF RX(169), RX(66)  
RX(325) LX + Z ==> GD

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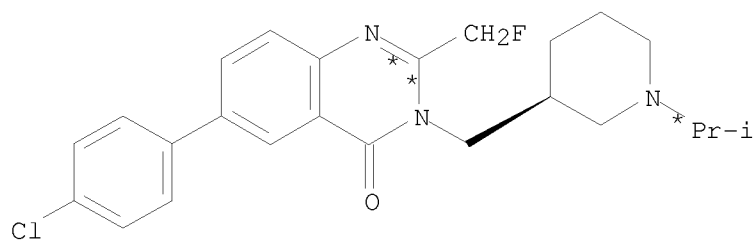


LX



Z

2  
STEPS  
→



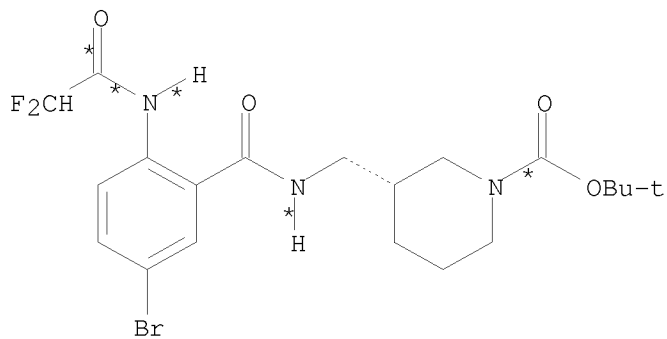
GD  
YIELD 27%

RX(169) RCT LX 875270-26-1  
RGT LY 109-63-7 BF<sub>3</sub>-Et<sub>2</sub>O  
PRO GC 875270-27-2  
SOL 64-19-7 AcOH  
CON 25 minutes, 130 deg C  
NTE microwave irradiation

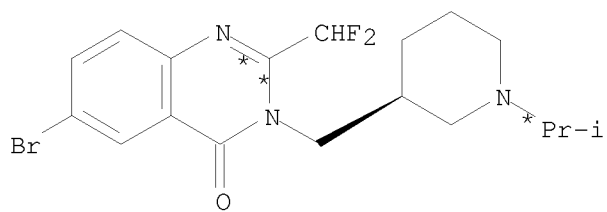
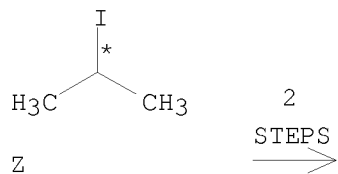
RX(66) RCT Z 75-30-9, GC 875270-27-2  
RGT AH 534-17-8 Cs<sub>2</sub>CO<sub>3</sub>  
PRO GD 875259-45-3  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) 15 hours, room temperature -> 70 deg C  
SUBSTAGE(2) 70 deg C -> room temperature

RX(327) OF 652 COMPOSED OF RX(171), RX(172)  
RX(327) MA + Z ==> GF

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MA



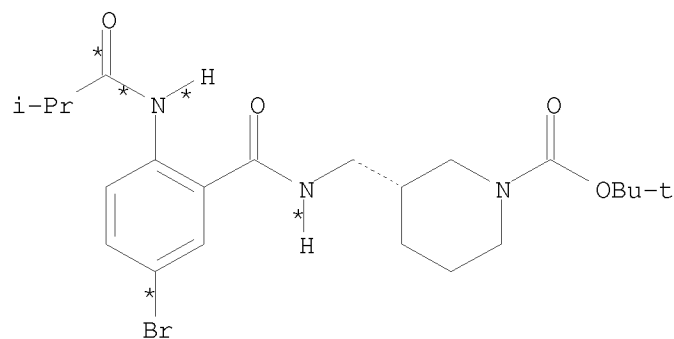
GF  
YIELD 81%

RX(171) RCT MA 875270-28-3  
PRO MD 875270-29-4  
SOL 64-19-7 AcOH  
CON 2 hours, 100 deg C  
NTE sealed vial used

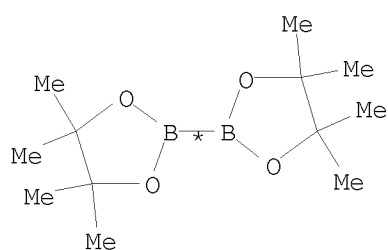
RX(172)      RCT    Z 75-30-9, MD 875270-29-4  
                  RGT    AB 584-08-7 K2CO3  
                  PRO    GF 875270-30-7  
                  SOL    75-05-8 MeCN  
                  CON    4 hours, 70 deg C

RX(461) OF 652 COMPOSED OF RX(137), RX(138), RX(139)  
RX(461) KT + KU ==> KX

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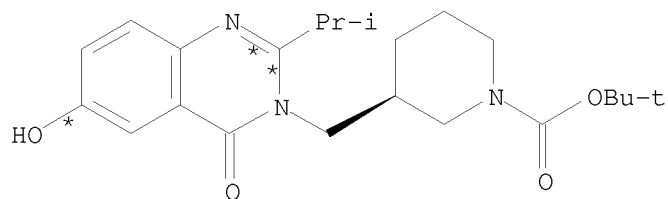


KT



KU

3  
STEPS  
→



KX

YIELD 88%

RX(137) RCT KT 875269-98-0  
RGT EB 1310-65-2 LiOH  
PRO KS 875269-86-6  
SOL 107-21-1 (CH<sub>2</sub>OH)<sub>2</sub>  
CON 15 hours, 130 deg C

RX(138) RCT KS 875269-86-6, KU 73183-34-3  
RGT KW 127-08-2 AcOK  
PRO KV 875269-87-7  
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-  
κP)ferrocene]dichloro-, (SP-4-2)-  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 2 minutes, room temperature  
SUBSTAGE(2) 15 hours, room temperature -> 60 deg C

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SUBSTAGE(3) 60 deg C -> room temperature  
NTE Suzuki coupling reaction

RX(139) RCT KV 875269-87-7

STAGE(1)

RGT E 1310-73-2 NaOH, KY 7722-84-1 H2O2  
SOL 7732-18-5 Water, 109-99-9 THF  
CON 1 hour, room temperature

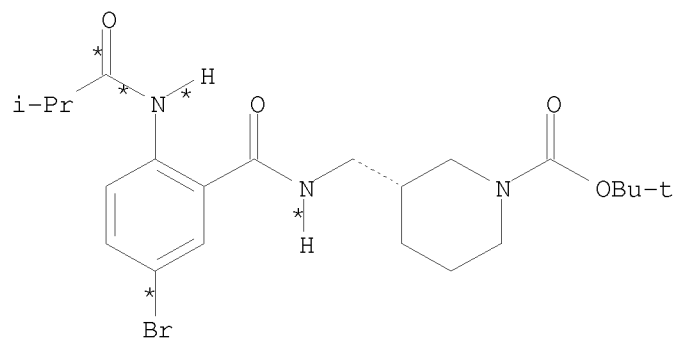
STAGE(2)

RGT CC 12125-02-9 NH4Cl  
SOL 7732-18-5 Water  
CON pH 7.0

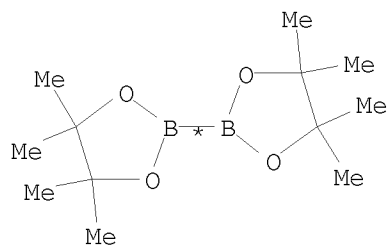
PRO KX 875269-88-8

RX(462) OF 652 COMPOSED OF RX(137), RX(138), RX(178)

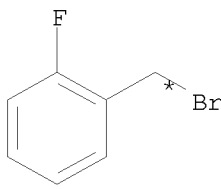
RX(462) KT + KU + MK ==> ML



KT



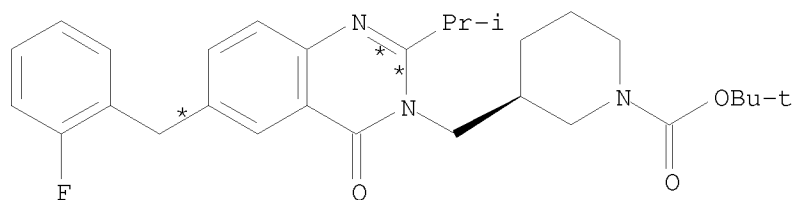
KU



MK

3  
STEPS  
→

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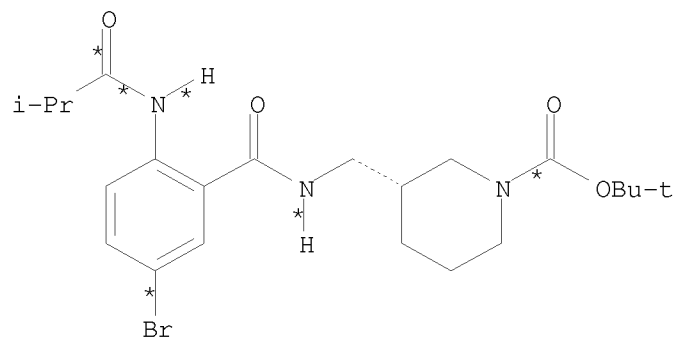
ML  
YIELD 71%

RX(137) RCT KT 875269-98-0  
RGT EB 1310-65-2 LiOH  
PRO KS 875269-86-6  
SOL 107-21-1 (CH<sub>2</sub>OH)<sub>2</sub>  
CON 15 hours, 130 deg C

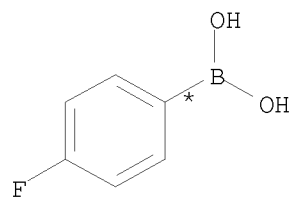
RX(138) RCT KS 875269-86-6, KU 73183-34-3  
RGT KW 127-08-2 AcOK  
PRO KV 875269-87-7  
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 2 minutes, room temperature  
SUBSTAGE(2) 15 hours, room temperature -> 60 deg C  
SUBSTAGE(3) 60 deg C -> room temperature  
NTE Suzuki coupling reaction

RX(178) RCT KV 875269-87-7, MK 446-48-0  
RGT AB 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO ML 875270-37-4  
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-  
SOL 123-91-1 Dioxane, 108-88-3 PhMe  
CON SUBSTAGE(1) 1 minute  
SUBSTAGE(2) 15 hours, 90 deg C  
SUBSTAGE(3) 90 deg C -> room temperature

RX(463) OF 652 COMPOSED OF RX(137), RX(151), RX(42)  
RX(463) KT + GE ==> DU

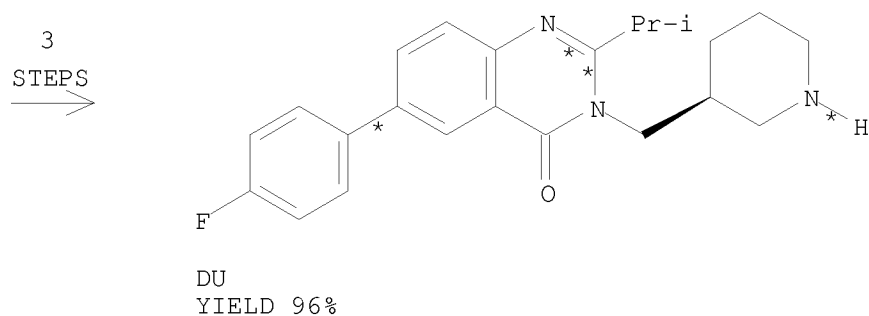


KT



GE



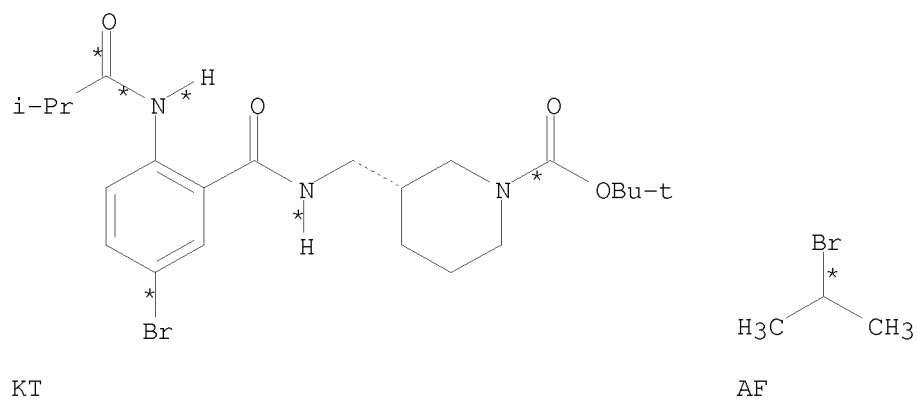


RX(137) RCT KT 875269-98-0  
RGT EB 1310-65-2 LiOH  
PRO KS 875269-86-6  
SOL 107-21-1 (CH<sub>2</sub>OH)<sub>2</sub>  
CON 15 hours, 130 deg C

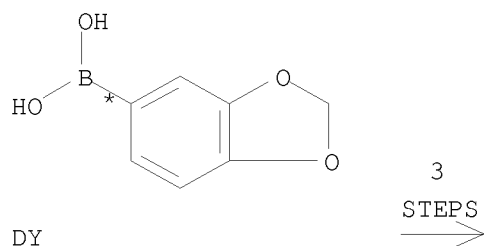
RX(151) RCT KS 875269-86-6, GE 1765-93-1  
RGT AB 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO DT 875269-99-1  
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-  
κP)ferrocene]dichloro-, (SP-4-2)-  
SOL 7732-18-5 Water, 123-91-1 Dioxane, 108-88-3 PhMe  
CON 15 hours, 80 deg C  
NTE Suzuki coupling reaction

RX(42) RCT DT 875269-99-1  
RGT C 76-05-1 F<sub>3</sub>CCO<sub>2</sub>H  
PRO DU 875259-16-8  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 15 hours, room temperature

RX(464) OF 652 COMPOSED OF RX(137), RX(157), RX(50)  
RX(464) KT + AF + DY ==> EU



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EU  
YIELD 56%

RX(137) RCT KT 875269-98-0  
RGT EB 1310-65-2 LiOH  
PRO KS 875269-86-6  
SOL 107-21-1 (CH<sub>2</sub>OH)<sub>2</sub>  
CON 15 hours, 130 deg C

RX(157) RCT KS 875269-86-6

STAGE(1)

RGT C 76-05-1 F<sub>3</sub>CCO<sub>2</sub>H  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 3 hours, room temperature

STAGE(2)

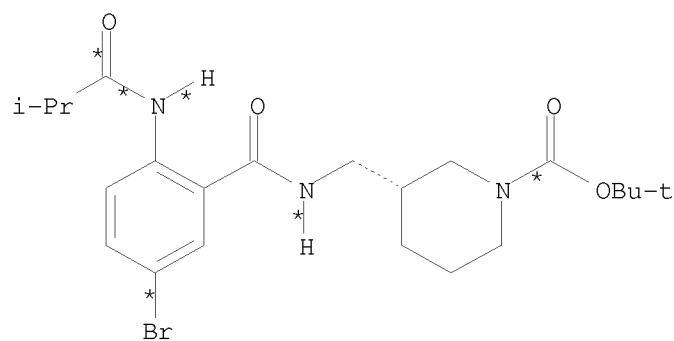
RCT AF 75-26-3  
RGT AH 534-17-8 Cs<sub>2</sub>CO<sub>3</sub>  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) 14 hours, 70 deg C  
SUBSTAGE(2) 70 deg C -> room temperature

PRO ET 875270-09-0

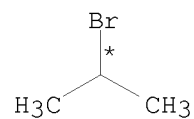
RX(50) RCT DY 94839-07-3, ET 875270-09-0  
RGT AB 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO EU 875259-29-3  
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-  
κP)ferrocene]dichloro-, (SP-4-2)-  
SOL 7732-18-5 Water, 127-19-5 AcNMe<sub>2</sub>  
CON SUBSTAGE(1) 15 minutes, 130 deg C  
SUBSTAGE(2) 130 deg C -> room temperature  
NTE microwave irradiation, Suzuki coupling reaction, sealed vial  
used

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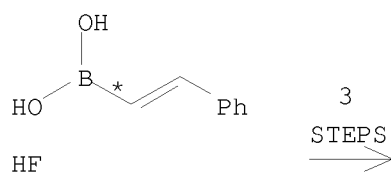
RX(465) OF 652 COMPOSED OF RX(137), RX(157), RX(77)  
RX(465) KT + AF + HF ==> HG



KT

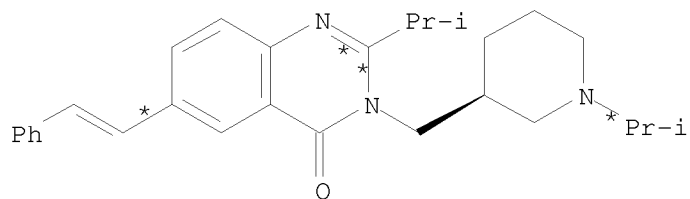


AF



HF

3  
STEPS  
→



HG

RX(137) RCT KT 875269-98-0  
RGT EB 1310-65-2 LiOH  
PRO KS 875269-86-6  
SOL 107-21-1 (CH2OH)2  
CON 15 hours, 130 deg C

RX(157) RCT KS 875269-86-6

STAGE(1)

RGT C 76-05-1 F3CCO2H  
SOL 75-09-2 CH2Cl2  
CON 3 hours, room temperature

STAGE(2)

RCT AF 75-26-3

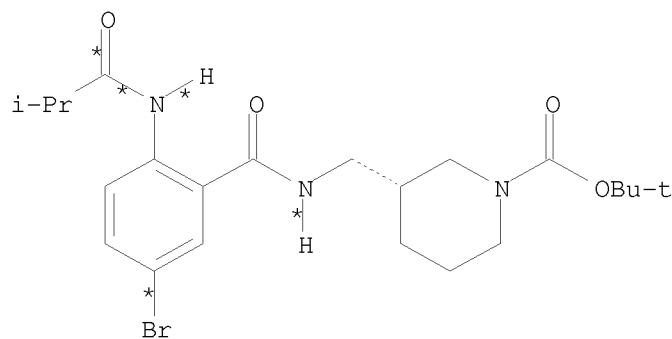
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RGT AH 534-17-8 Cs2CO3  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) 14 hours, 70 deg C  
SUBSTAGE(2) 70 deg C -> room temperature

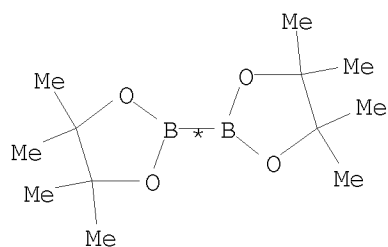
PRO ET 875270-09-0

RX(77) RCT ET 875270-09-0, HF 6783-05-7  
RGT AB 584-08-7 K2CO3  
PRO HG 875259-62-4  
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-  
κP)ferrocene]dichloro-, (SP-4-2)-  
SOL 7732-18-5 Water, 127-19-5 AcNMe2  
CON SUBSTAGE(1) 15 minutes, 130 deg C  
SUBSTAGE(2) 130 deg C -> room temperature  
NTE stereoselective, microwave irradiation, sealed tube used, Suzuki  
coupling reaction

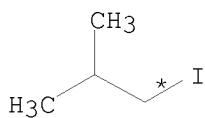
RX(480) OF 652 COMPOSED OF RX(137), RX(138), RX(139), RX(140)  
RX(480) KT + KU + KE ==> KZ



KT



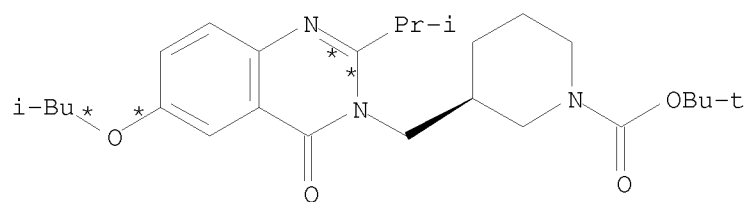
KU



KE

4  
STEPS  
→

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KZ  
YIELD 74%

RX(137) RCT KT 875269-98-0  
RGT EB 1310-65-2 LiOH  
PRO KS 875269-86-6  
SOL 107-21-1 (CH<sub>2</sub>OH)<sub>2</sub>  
CON 15 hours, 130 deg C

RX(138) RCT KS 875269-86-6, KU 73183-34-3  
RGT KW 127-08-2 AcOK  
PRO KV 875269-87-7  
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 2 minutes, room temperature  
SUBSTAGE(2) 15 hours, room temperature -> 60 deg C  
SUBSTAGE(3) 60 deg C -> room temperature  
NTE Suzuki coupling reaction

RX(139) RCT KV 875269-87-7

STAGE(1)  
RGT E 1310-73-2 NaOH, KY 7722-84-1 H<sub>2</sub>O<sub>2</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON 1 hour, room temperature

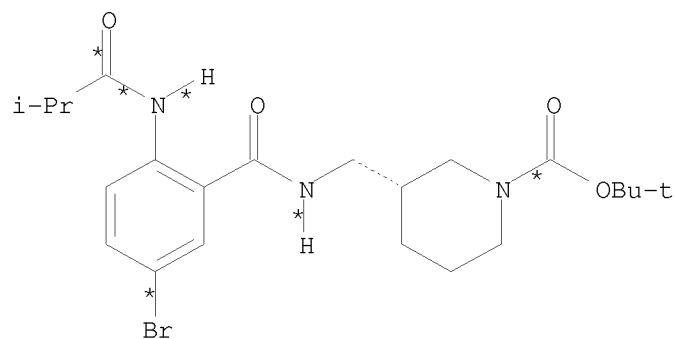
STAGE(2)  
RGT CC 12125-02-9 NH<sub>4</sub>Cl  
SOL 7732-18-5 Water  
CON pH 7.0

PRO KX 875269-88-8

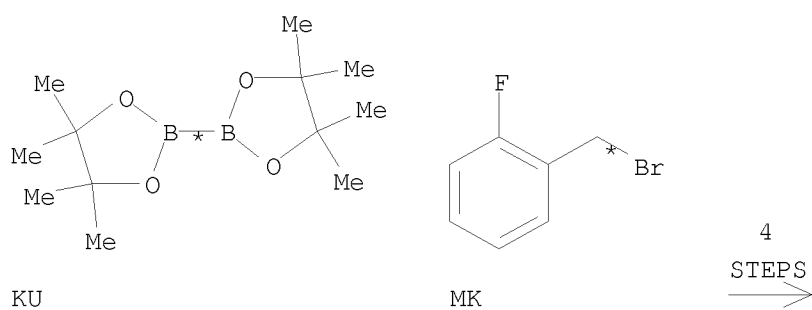
RX(140) RCT KE 513-38-2, KX 875269-88-8  
RGT AH 534-17-8 Cs<sub>2</sub>CO<sub>3</sub>  
PRO KZ 875269-89-9  
SOL 68-12-2 DMF  
CON 15 hours, 90 deg C

RX(481) OF 652 COMPOSED OF RX(137), RX(138), RX(178), RX(179)  
RX(481) KT + KU + MK ==> HK

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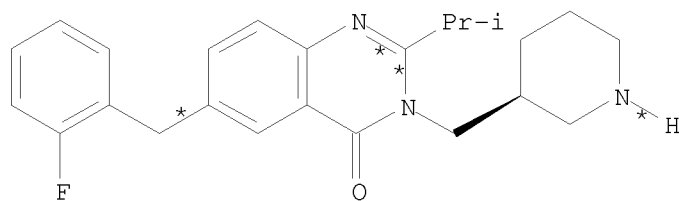


KT



KU

MK



HK

YIELD 87%

RX(137) RCT KT 875269-98-0  
RGT EB 1310-65-2 LiOH  
PRO KS 875269-86-6  
SOL 107-21-1 (CH<sub>2</sub>OH)<sub>2</sub>  
CON 15 hours, 130 deg C

RX(138) RCT KS 875269-86-6, KU 73183-34-3  
RGT KW 127-08-2 AcOK  
PRO KV 875269-87-7  
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-  
κP)ferrocene]dichloro-, (SP-4-2)-  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 2 minutes, room temperature  
SUBSTAGE(2) 15 hours, room temperature -> 60 deg C

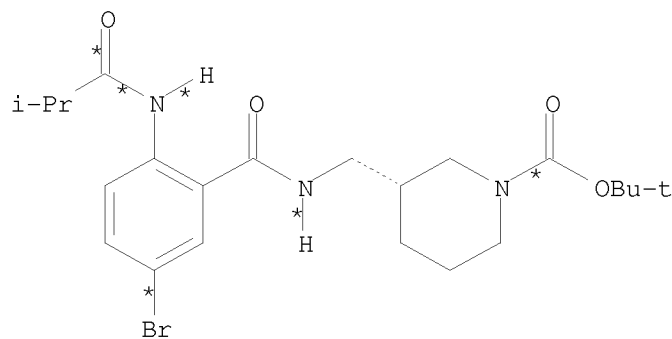
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SUBSTAGE(3) 60 deg C -> room temperature  
NTE Suzuki coupling reaction

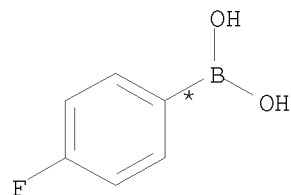
RX(178) RCT KV 875269-87-7, MK 446-48-0  
RGT AB 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO ML 875270-37-4  
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-  
κP)ferrocene]dichloro-, (SP-4-2)-  
SOL 123-91-1 Dioxane, 108-88-3 PhMe  
CON SUBSTAGE(1) 1 minute  
SUBSTAGE(2) 15 hours, 90 deg C  
SUBSTAGE(3) 90 deg C -> room temperature

RX(179) RCT ML 875270-37-4  
RGT C 76-05-1 F<sub>3</sub>CCO<sub>2</sub>H  
PRO HK 875270-38-5  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 15 hours, room temperature

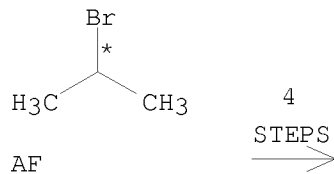
RX(509) OF 652 COMPOSED OF RX(137), RX(151), RX(42), RX(43)  
RX(509) KT + GE + AF ==> DV



KT

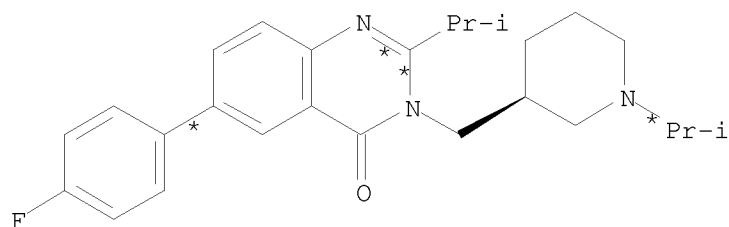


GE



AF

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DV  
YIELD 77%

RX(137) RCT KT 875269-98-0  
RGT EB 1310-65-2 LiOH  
PRO KS 875269-86-6  
SOL 107-21-1 (CH<sub>2</sub>OH)<sub>2</sub>  
CON 15 hours, 130 deg C

RX(151) RCT KS 875269-86-6, GE 1765-93-1  
RGT AB 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO DT 875269-99-1  
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-  
SOL 7732-18-5 Water, 123-91-1 Dioxane, 108-88-3 PhMe  
CON 15 hours, 80 deg C  
NTE Suzuki coupling reaction

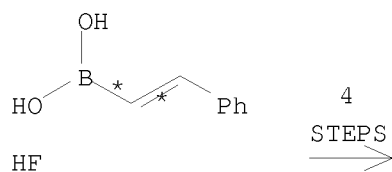
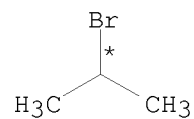
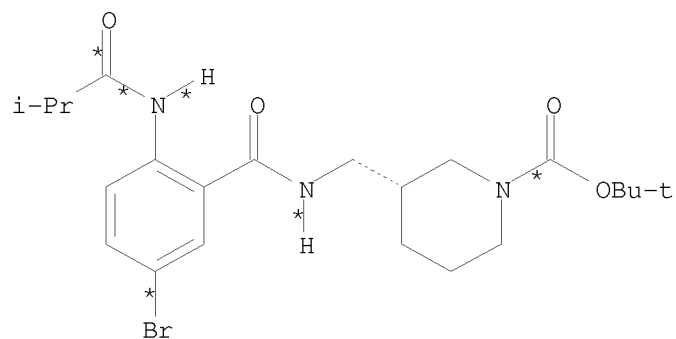
RX(42) RCT DT 875269-99-1  
RGT C 76-05-1 F<sub>3</sub>CCO<sub>2</sub>H  
PRO DU 875259-16-8  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 15 hours, room temperature

RX(43) RCT DU 875259-16-8, AF 75-26-3  
RGT AB 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO DV 875259-17-9  
SOL 75-05-8 MeCN  
CON 4 hours, 70 deg C

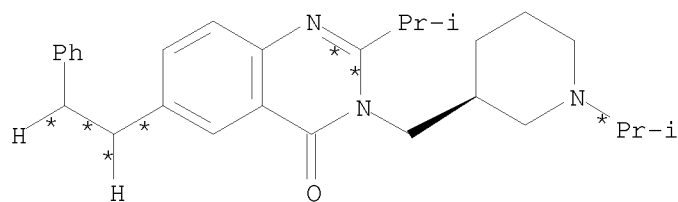
RX(515) OF 652 COMPOSED OF RX(137), RX(157), RX(77), RX(78)  
RX(515) KT + AF + HF ==> HH



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4  
STEPS  
→



YIELD 90%

RX(137) RCT KT 875269-98-0  
RGT EB 1310-65-2 LiOH  
PRO KS 875269-86-6  
SOL 107-21-1 (CH<sub>2</sub>OH)<sub>2</sub>  
CON 15 hours, 130 deg C

RX(157) RCT KS 875269-86-6

STAGE(1)

RGT C 76-05-1 F<sub>3</sub>CCO<sub>2</sub>H  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 3 hours, room temperature

STAGE(2)

RCT AF 75-26-3  
RGT AH 534-17-8 Cs<sub>2</sub>CO<sub>3</sub>  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) 14 hours, 70 deg C  
SUBSTAGE(2) 70 deg C -> room temperature

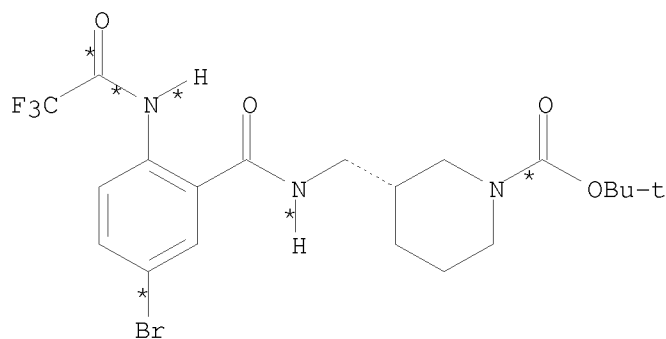
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PRO ET 875270-09-0

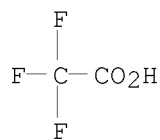
RX(77) RCT ET 875270-09-0, HF 6783-05-7  
RGT AB 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO HG 875259-62-4  
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-  
κP)ferrocene]dichloro-, (SP-4-2)-  
SOL 7732-18-5 Water, 127-19-5 AcNMe<sub>2</sub>  
CON SUBSTAGE(1) 15 minutes, 130 deg C  
SUBSTAGE(2) 130 deg C -> room temperature  
NTE stereoselective, microwave irradiation, sealed tube used, Suzuki  
coupling reaction

RX(78) RCT HG 875259-62-4  
RGT HA 1333-74-0 H<sub>2</sub>  
PRO HH 875259-63-5  
CAT 7440-05-3 Pd  
SOL 67-56-1 MeOH  
CON 3 hours, room temperature

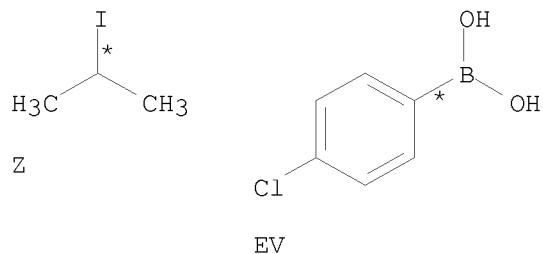
RX(526) OF 652 COMPOSED OF RX(164), RX(165), RX(58)  
RX(526) LR + C + Z + EV ==> FO



LR

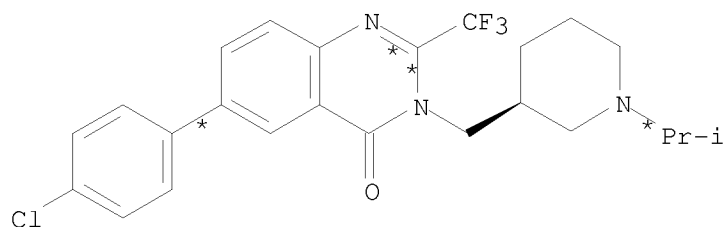


C



3  
STEPS  
→

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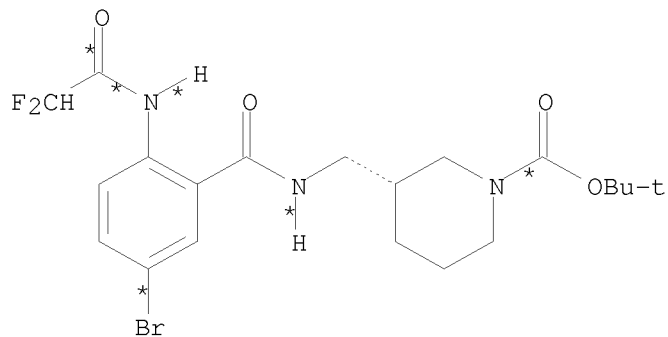
FO  
YIELD 86%

RX(164) RCT LR 875270-16-9, C 76-05-1  
PRO LS 875270-18-1  
CON 1 hour, 150 deg C  
NTE microwave irradiation

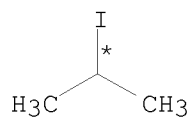
RX(165) RCT Z 75-30-9, LS 875270-18-1  
RGT AB 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO FN 875270-20-5  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 15 hours, room temperature -> 70 deg C  
SUBSTAGE(3) 70 deg C -> room temperature

RX(58) RCT EV 1679-18-1, FN 875270-20-5  
RGT FC 312959-24-3 Ferrocene,  
1'-[bis(1,1-dimethylethyl)phosphino]-1,2,3,4,5-pentaphenyl-, FD  
13400-13-0 CsF  
PRO FO 875259-37-3  
CAT 52522-40-4 Pd complex  
SOL 109-99-9 THF  
CON 12 hours, room temperature  
NTE Suzuki coupling reaction

RX(535) OF 652 COMPOSED OF RX(171), RX(172), RX(67)  
RX(535) MA + Z + GE ==> GG

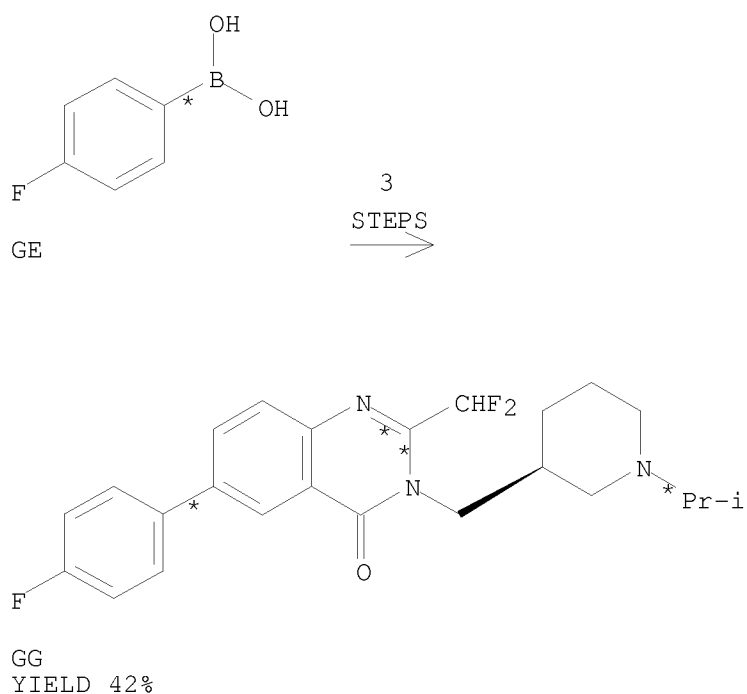


MA



Z

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RX(171) RCT MA 875270-28-3  
PRO MD 875270-29-4  
SOL 64-19-7 AcOH  
CON 2 hours, 100 deg C  
NTE sealed vial used

RX(172) RCT Z 75-30-9, MD 875270-29-4  
RGT AB 584-08-7 K2CO3  
PRO GF 875270-30-7  
SOL 75-05-8 MeCN  
CON 4 hours, 70 deg C

RX(67) RCT GE 1765-93-1, GF 875270-30-7

STAGE(1)

RGT FD 13400-13-0 CsF  
SOL 109-99-9 THF  
CON 20 minutes

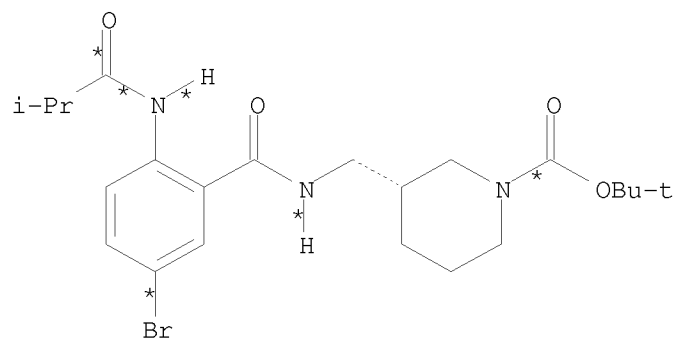
STAGE(2)

RGT FC 312959-24-3 Ferrocene,  
1'-[bis(1,1-dimethylethyl)phosphino]-1,2,3,4,5-pentaphenyl-  
CAT 52522-40-4 Pd complex  
CON 10 hours, room temperature

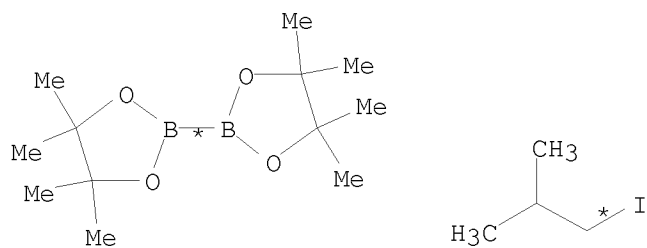
PRO GG 875259-46-4  
NTE Suzuki coupling reaction

RX(626) OF 652 COMPOSED OF RX(137), RX(138), RX(139), RX(140), RX(141)  
RX(626) KT + KU + KE ==> CS

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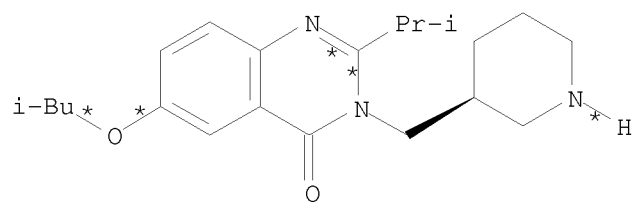
KT



KU



KE



CS  
YIELD 79%

RX(137) RCT KT 875269-98-0  
RGT EB 1310-65-2 LiOH  
PRO KS 875269-86-6  
SOL 107-21-1 (CH<sub>2</sub>OH)<sub>2</sub>  
CON 15 hours, 130 deg C

RX(138) RCT KS 875269-86-6, KU 73183-34-3  
RGT KW 127-08-2 AcOK  
PRO KV 875269-87-7  
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 2 minutes, room temperature

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SUBSTAGE(2) 15 hours, room temperature -> 60 deg C  
SUBSTAGE(3) 60 deg C -> room temperature  
NTE Suzuki coupling reaction

RX(139) RCT KV 875269-87-7

STAGE(1)

RGT E 1310-73-2 NaOH, KY 7722-84-1 H2O2  
SOL 7732-18-5 Water, 109-99-9 THF  
CON 1 hour, room temperature

STAGE(2)

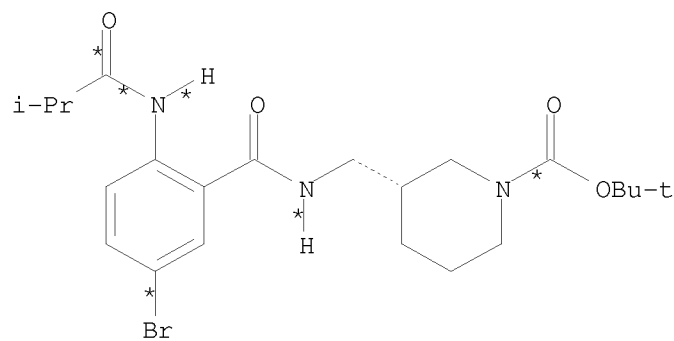
RGT CC 12125-02-9 NH4Cl  
SOL 7732-18-5 Water  
CON pH 7.0

PRO KX 875269-88-8

RX(140) RCT KE 513-38-2, KX 875269-88-8  
RGT AH 534-17-8 Cs2CO3  
PRO KZ 875269-89-9  
SOL 68-12-2 DMF  
CON 15 hours, 90 deg C

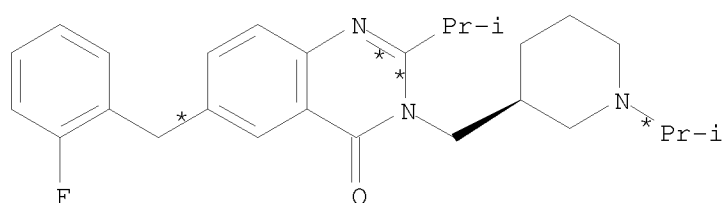
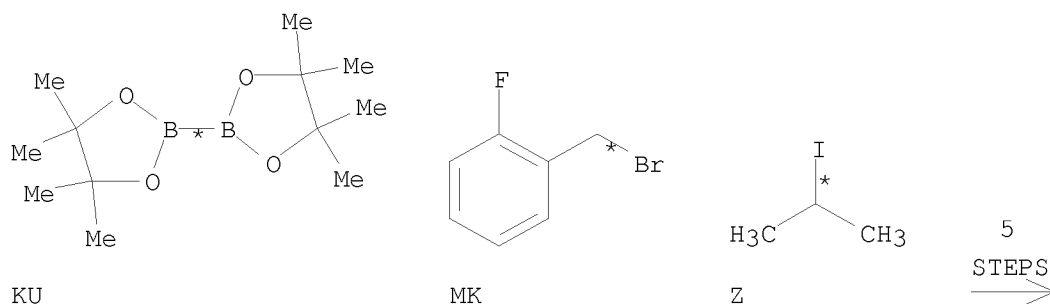
RX(141) RCT KZ 875269-89-9  
RGT C 76-05-1 F3CCO2H  
PRO CS 875269-90-2  
SOL 75-09-2 CH2Cl2  
CON 15 hours, room temperature

RX(627) OF 652 COMPOSED OF RX(137), RX(138), RX(178), RX(179), RX(80)  
RX(627) KT + KU + MK + Z ==> HL



KT

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HL  
YIELD 11%

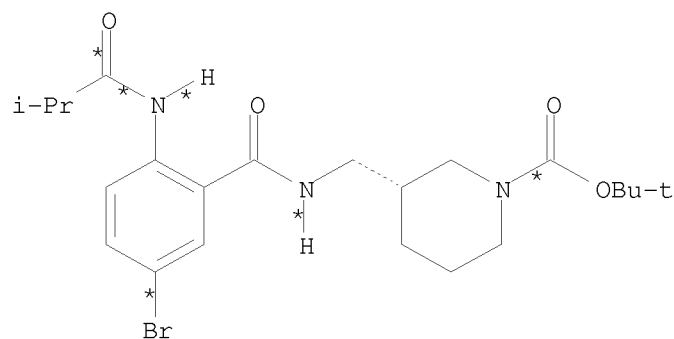
RX(137)	RCT	KT 875269-98-0
	RGT	EB 1310-65-2 LiOH
	PRO	KS 875269-86-6
	SOL	107-21-1 (CH <sub>2</sub> OH) <sub>2</sub>
	CON	15 hours, 130 deg C
RX(138)	RCT	KS 875269-86-6, KU 73183-34-3
	RGT	KW 127-08-2 AcOK
	PRO	KV 875269-87-7
	CAT	72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-
	SOL	68-12-2 DMF
	CON	SUBSTAGE(1) 2 minutes, room temperature SUBSTAGE(2) 15 hours, room temperature -> 60 deg C SUBSTAGE(3) 60 deg C -> room temperature
	NTE	Suzuki coupling reaction
RX(178)	RCT	KV 875269-87-7, MK 446-48-0
	RGT	AB 584-08-7 K <sub>2</sub> CO <sub>3</sub>
	PRO	ML 875270-37-4
	CAT	72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-
	SOL	123-91-1 Dioxane, 108-88-3 PhMe
	CON	SUBSTAGE(1) 1 minute SUBSTAGE(2) 15 hours, 90 deg C SUBSTAGE(3) 90 deg C -> room temperature
RX(179)	RCT	ML 875270-37-4
	RGT	C 76-05-1 F <sub>3</sub> CCO <sub>2</sub> H
	PRO	HK 875270-38-5
	SOL	75-09-2 CH <sub>2</sub> Cl <sub>2</sub>

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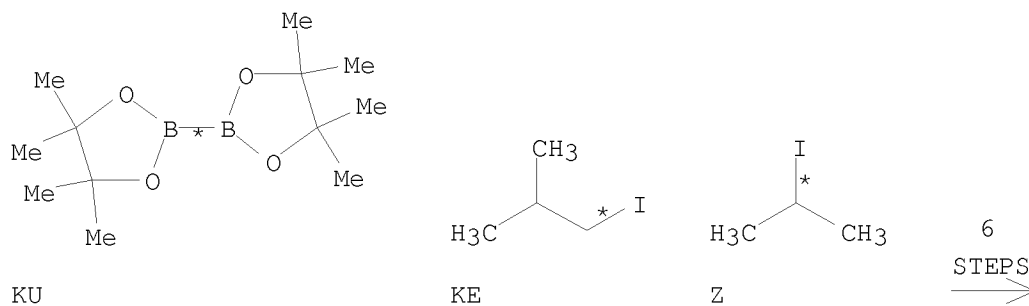
CON 15 hours, room temperature

RX(80) RCT Z 75-30-9, HK 875270-38-5  
RGT AH 534-17-8 Cs2CO3  
PRO HL 875259-65-7  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) 15 hours, room temperature -> 90 deg C  
SUBSTAGE(2) 90 deg C -> room temperature

RX(644) OF 652 COMPOSED OF RX(137), RX(138), RX(139), RX(140), RX(141), RX(33)  
RX(644) KT + KU + KE + Z ==> CT



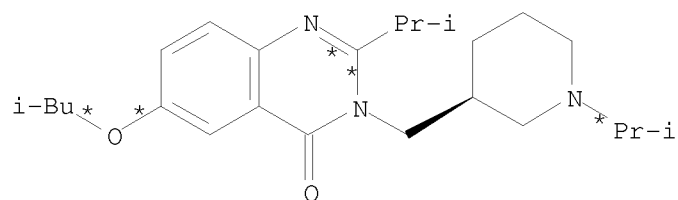
KT



KU

KE

Z



CT  
YIELD 30%

RX(137) RCT KT 875269-98-0



RGT EB 1310-65-2 LiOH  
PRO KS 875269-86-6  
SOL 107-21-1 (CH<sub>2</sub>OH)<sub>2</sub>  
CON 15 hours, 130 deg C

RX(138) RCT KS 875269-86-6, KU 73183-34-3  
RGT KW 127-08-2 AcOK  
PRO KV 875269-87-7  
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-  
κP)ferrocene]dichloro-, (SP-4-2)-  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 2 minutes, room temperature  
SUBSTAGE(2) 15 hours, room temperature -> 60 deg C  
SUBSTAGE(3) 60 deg C -> room temperature  
NTE Suzuki coupling reaction

RX(139) RCT KV 875269-87-7

STAGE(1)  
RGT E 1310-73-2 NaOH, KY 7722-84-1 H<sub>2</sub>O<sub>2</sub>  
SOL 7732-18-5 Water, 109-99-9 THF  
CON 1 hour, room temperature

STAGE(2)  
RGT CC 12125-02-9 NH<sub>4</sub>Cl  
SOL 7732-18-5 Water  
CON pH 7.0

PRO KX 875269-88-8

RX(140) RCT KE 513-38-2, KX 875269-88-8  
RGT AH 534-17-8 Cs<sub>2</sub>CO<sub>3</sub>  
PRO KZ 875269-89-9  
SOL 68-12-2 DMF  
CON 15 hours, 90 deg C

RX(141) RCT KZ 875269-89-9  
RGT C 76-05-1 F<sub>3</sub>CCO<sub>2</sub>H  
PRO CS 875269-90-2  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 15 hours, room temperature

RX(33) RCT Z 75-30-9, CS 875269-90-2  
RGT AH 534-17-8 Cs<sub>2</sub>CO<sub>3</sub>  
PRO CT 875259-02-2  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) 15 hours, room temperature -> 90 deg C  
SUBSTAGE(2) 90 deg C -> room temperature

L3 ANSWER 41 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

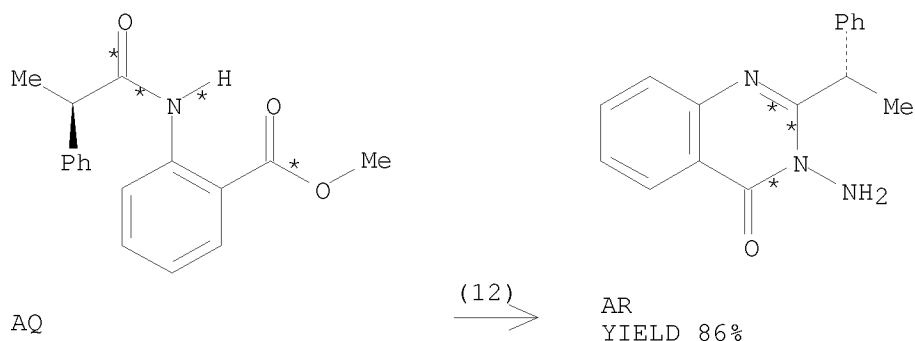
ACCESSION NUMBER: 144:166375 CASREACT

TITLE: The stereoselective synthesis of aziridine analogues  
of diaminopimelic acid (DAP) and their interaction  
with DAP epimeraseAUTHOR(S): Diaper, Christopher M.; Sutherland, Andrew; Pillai,  
Bindu; James, Michael N. G.; Semchuk, Paul; Blanchard,

CORPORATE SOURCE: John S.; Vederas, John C.  
 Department of Chemistry, University of Alberta,  
 Edmonton, AB, T6G 2G2, Can.  
 SOURCE: Organic & Biomolecular Chemistry (2005), 3(24),  
 4402-4411  
 CODEN: OBCRAK; ISSN: 1477-0520  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Aziridine analogs of diaminopimelic acid (DAP) have been prepared stereoselectively for the first time and evaluated as inhibitors of DAP epimerase. (2R,3S,3'S)-3-(3'-Aminopropyl)aziridine-2,3'-dicarboxylate 4 was synthesized and shown to be a reversible inhibitor of DAP epimerase with an IC<sub>50</sub> value of 2.88 mM. (2S,4S)- and (2S,4R)-2-(4-Amino-4-carboxybutyl)aziridine-2-carboxylic acid (LL-azi-DAP 14 and DL-azi-DAP 29) were made as pure diastereomers, and both were shown to be irreversible inhibitors of DAP epimerase. LL-Azi-DAP 14 selectively binds to Cys-73 of the enzyme active site whereas DL-azi-DAP 29 binds to Cys-217 via attack of sulfhydryl on the methylene of the inhibitor aziridine ring. These observations are consistent with the two base mechanism proposed for the epimerization of LL-DAP 1 and meso-DAP 2 by DAP epimerase.

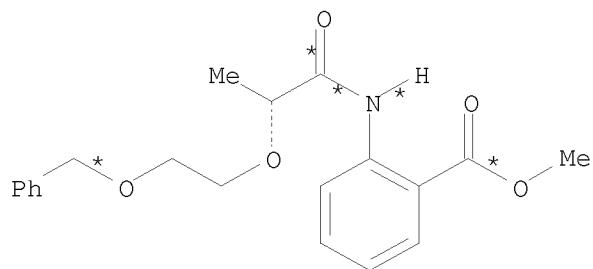
RX(12) OF 122 ...AQ ==> AR



RX(12) RCT AQ 923014-08-8  
 RGT AS 7803-57-8 N2H4-H2O  
 PRO AR 874534-88-0  
 SOL 64-17-5 EtOH  
 CON 16 hours, 140 deg C  
 NTE sealed tube used

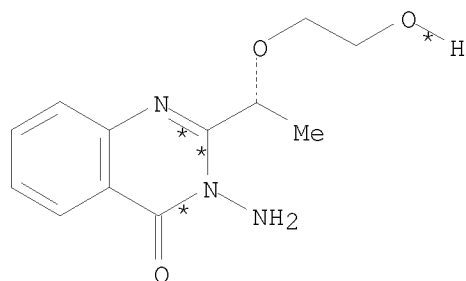
RX(13) OF 122 ...AT ==> AU...

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AT

(13)  $\longrightarrow$



AU

YIELD 69%

RX(13) RCT AT 445397-16-0

STAGE(1)

RGT AV 1333-74-0 H2

CAT 7440-05-3 Pd

SOL 67-56-1 MeOH

CON 19 hours, room temperature

STAGE(2)

RGT AW 302-01-2 N2H4

SOL 64-17-5 EtOH

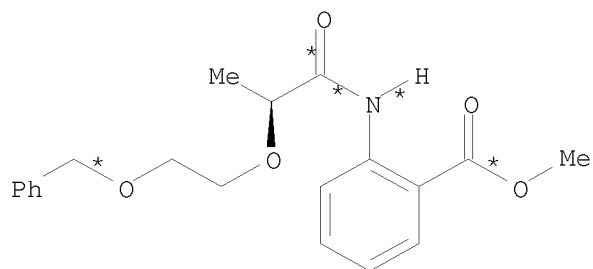
CON 2 hours, 140 deg C

PRO AU 445397-14-8

NTE sealed tube in 2nd stage

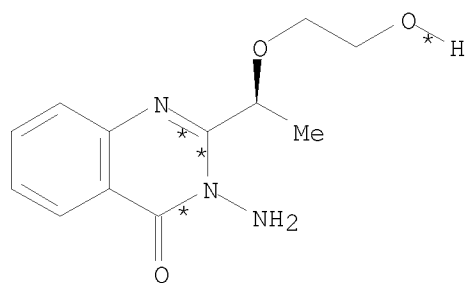
RX(14) OF 122 AY ==> AZ...

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AY

(14)  $\longrightarrow$



AZ

RX(14) RCT AY 923015-23-0

STAGE(1)

RGT AV 1333-74-0 H<sub>2</sub>

CAT 7440-05-3 Pd

SOL 67-56-1 MeOH

CON 19 hours, room temperature

STAGE(2)

RGT AW 302-01-2 N<sub>2</sub>H<sub>4</sub>

SOL 64-17-5 EtOH

CON 2 hours, 140 deg C

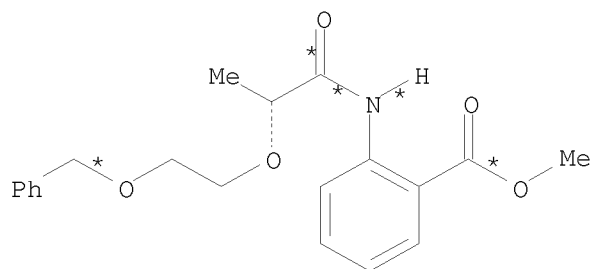
PRO AZ 874534-89-1

NTE sealed tube in 2nd stage

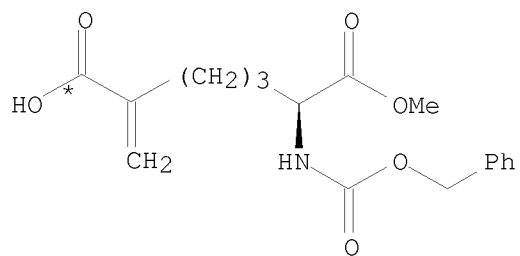
RX(44) OF 122 COMPOSED OF RX(13), RX(16)

RX(44) AT + BB ==> BD

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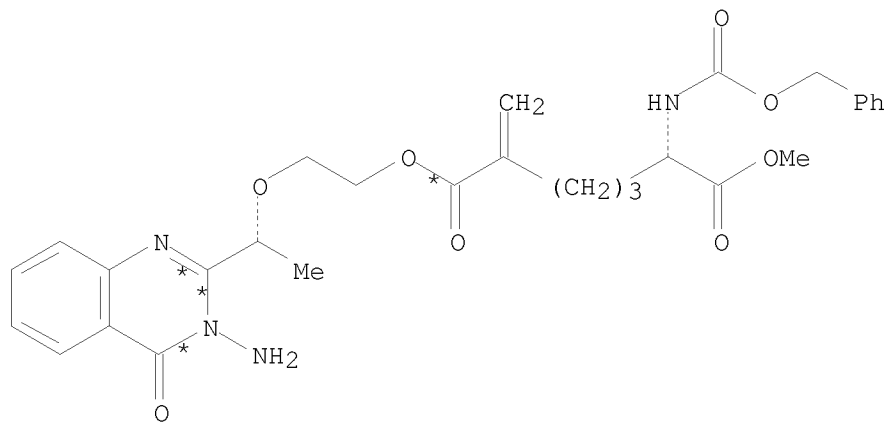


AT



BB

2  
STEPS  
→



BD

YIELD 62%

RX(13) RCT AT 445397-16-0

STAGE(1)

RGT AV 1333-74-0 H2

CAT 7440-05-3 Pd

SOL 67-56-1 MeOH

CON 19 hours, room temperature

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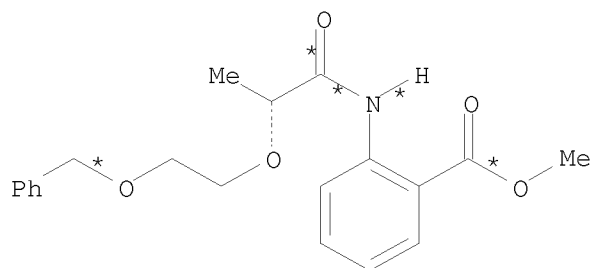
STAGE(2)

RGT AW 302-01-2 N2H4  
SOL 64-17-5 EtOH  
CON 2 hours, 140 deg C

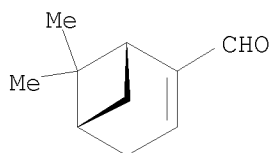
PRO AU 445397-14-8  
NTE sealed tube in 2nd stage

RX(16) RCT AU 445397-14-8, BB 874534-90-4  
RGT BE 538-75-0 DCC  
PRO BD 874534-91-5  
CAT 1122-58-3 4-DMAP  
SOL 75-09-2 CH2Cl2  
CON 1 hour, room temperature

RX(45) OF 122 COMPOSED OF RX(13), RX(32)  
RX(45) AT + CG ==> CH

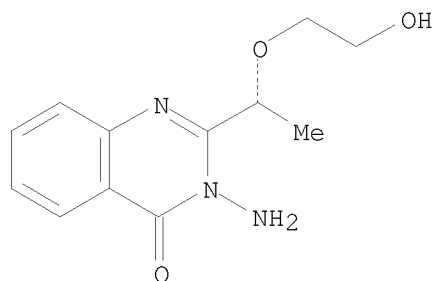


AT



CG

2  
STEPS  
→



CH  
YIELD 89%  
(-)-Myrtenal c  
onjugates

RX(13) RCT AT 445397-16-0

STAGE(1)

RGT AV 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 67-56-1 MeOH

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CON 19 hours, room temperature

STAGE(2)

RGT AW 302-01-2 N2H4

SOL 64-17-5 EtOH

CON 2 hours, 140 deg C

PRO AU 445397-14-8

NTE sealed tube in 2nd stage

RX(32) RCT AU 445397-14-8, CG 18486-69-6

RGT CI 64-19-7 AcOH

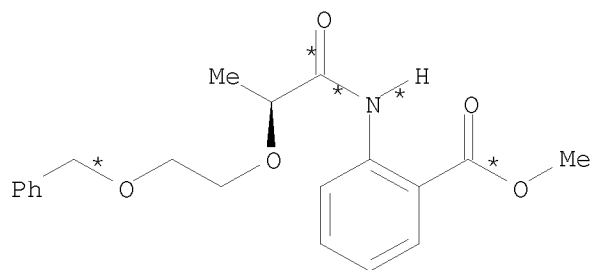
PRO CH 445397-14-8D

SOL 64-17-5 EtOH

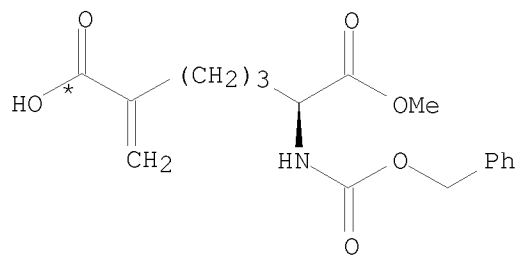
CON 16 hours, 70 deg C

RX(46) OF 122 COMPOSED OF RX(14), RX(18)

RX(46) AY + BB ==> BG



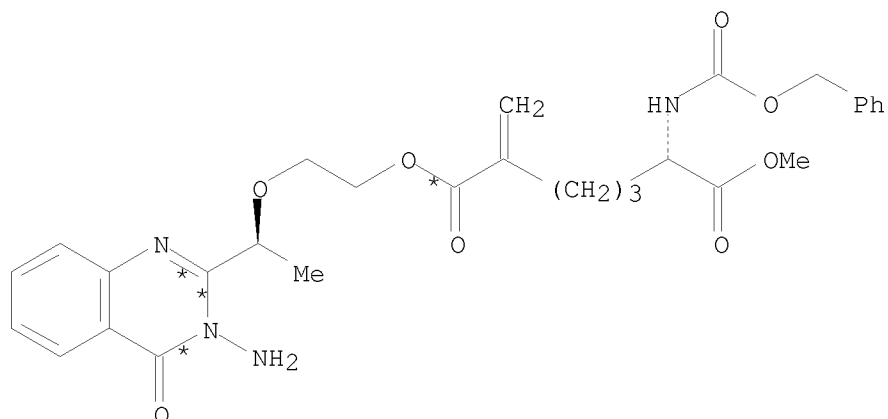
AY



BB

2  
STEPS  
=>

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BG  
YIELD 51%

RX(14) RCT AY 923015-23-0

STAGE(1)

RGT AV 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 67-56-1 MeOH  
CON 19 hours, room temperature

STAGE(2)

RGT AW 302-01-2 N2H4  
SOL 64-17-5 EtOH  
CON 2 hours, 140 deg C

PRO AZ 874534-89-1  
NTE sealed tube in 2nd stage

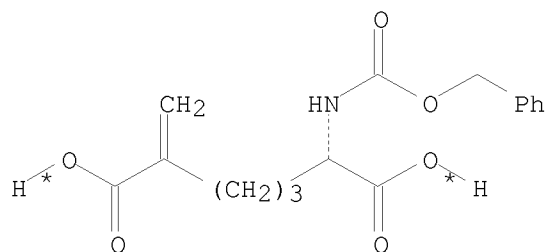
RX(18) RCT AZ 874534-89-1, BB 874534-90-4  
RGT BH 64075-39-4D Benzenemethanamine, N-(cyclohexylcarbonimidoyl)-  
PRO BG 874534-93-7  
CAT 1122-58-3 4-DMAP  
SOL 75-09-2 CH2Cl2  
CON 48 hours, room temperature  
NTE solid-supported reagent

RX(73) OF 122 COMPOSED OF REACTION SEQUENCE RX(15), RX(16)  
AND REACTION SEQUENCE RX(13), RX(16)

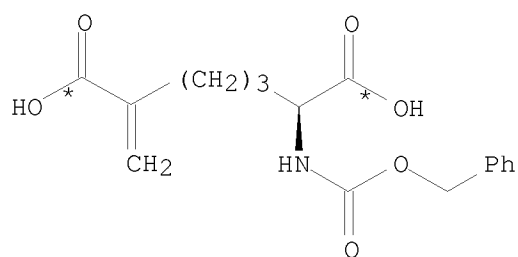
...2 BA + 3 M ==> BB...  
... AT + BB ==> BD



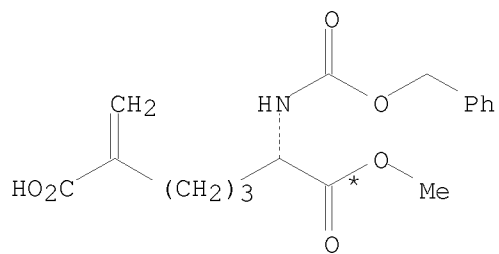
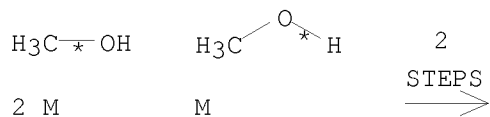
10/ 562,112



BA

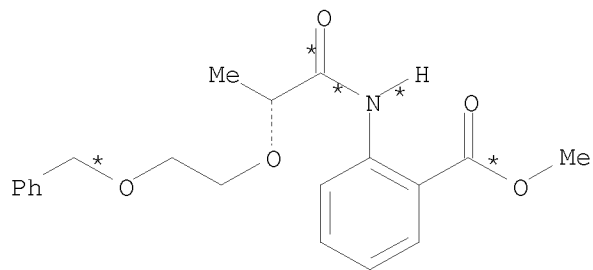


BA



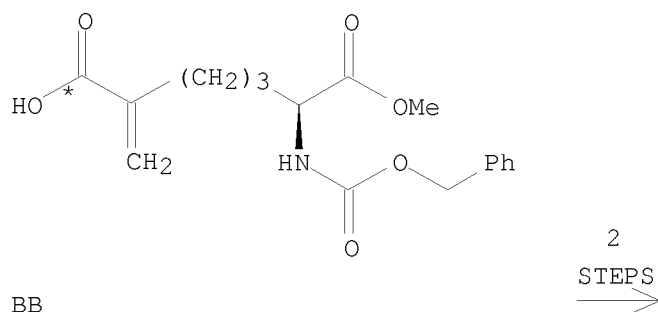
BB

START NEXT REACTION SEQUENCE

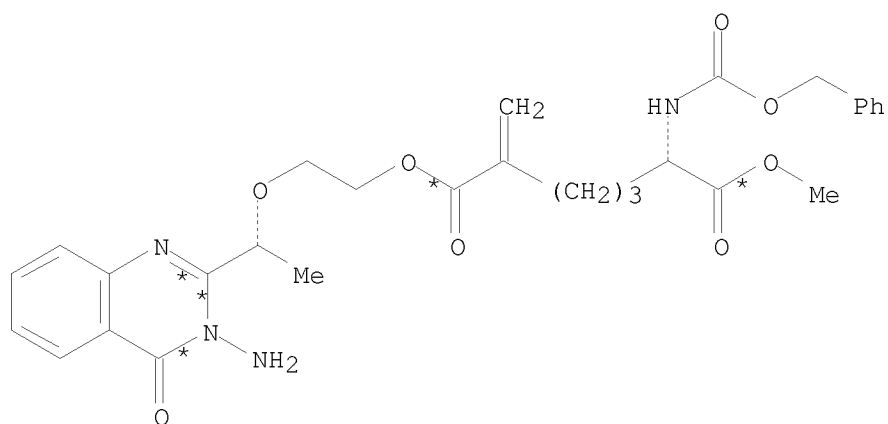


AT

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BB



BD

YIELD 62%

RX(15)    RCT    BA 874535-03-2, M 67-56-1  
          RGT    BC 104-15-4 TsOH  
          PRO    AF 874534-85-7, BB 874534-90-4  
          SOL    67-56-1 MeOH  
          CON    16 hours, room temperature  
          NTE    solid-supported reagent, 100% overall yield

RX(13)    RCT    AT 445397-16-0

STAGE(1)

          RGT    AV 1333-74-0 H<sub>2</sub>  
          CAT    7440-05-3 Pd  
          SOL    67-56-1 MeOH  
          CON    19 hours, room temperature

STAGE(2)

          RGT    AW 302-01-2 N<sub>2</sub>H<sub>4</sub>  
          SOL    64-17-5 EtOH  
          CON    2 hours, 140 deg C

          PRO    AU 445397-14-8  
          NTE    sealed tube in 2nd stage

RX(16)    RCT    AU 445397-14-8, BB 874534-90-4

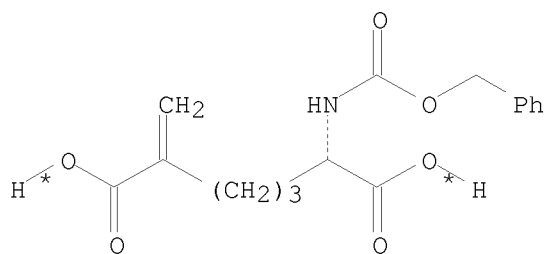
10/ 562,112

RGT BE 538-75-0 DCC  
PRO BD 874534-91-5  
CAT 1122-58-3 4-DMAP  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 1 hour, room temperature

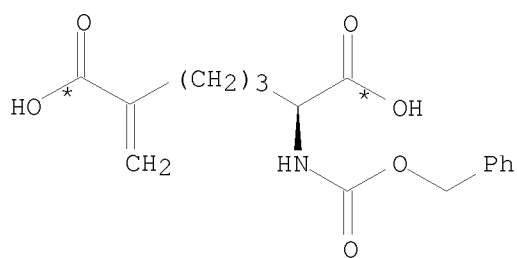
RX(77) OF 122 COMPOSED OF REACTION SEQUENCE RX(15), RX(18)  
AND REACTION SEQUENCE RX(14), RX(18)

...2 BA + 3 M ==> BB...

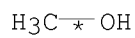
... AY + BB ==> BG



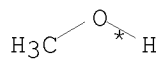
BA



BA

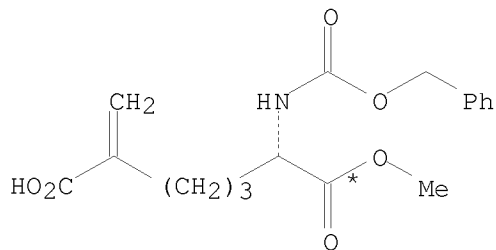


2 M



M

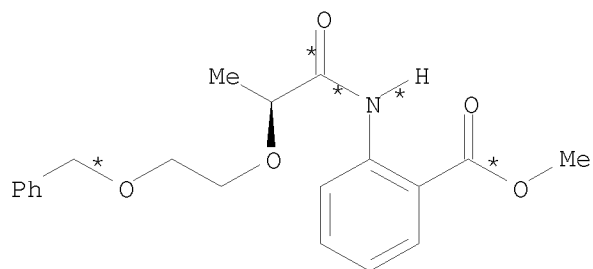
2  
STEPS  
→



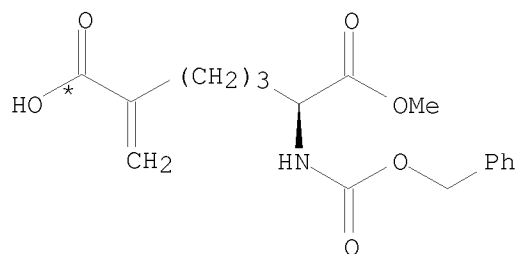
BB

START NEXT REACTION SEQUENCE

10/ 562,112

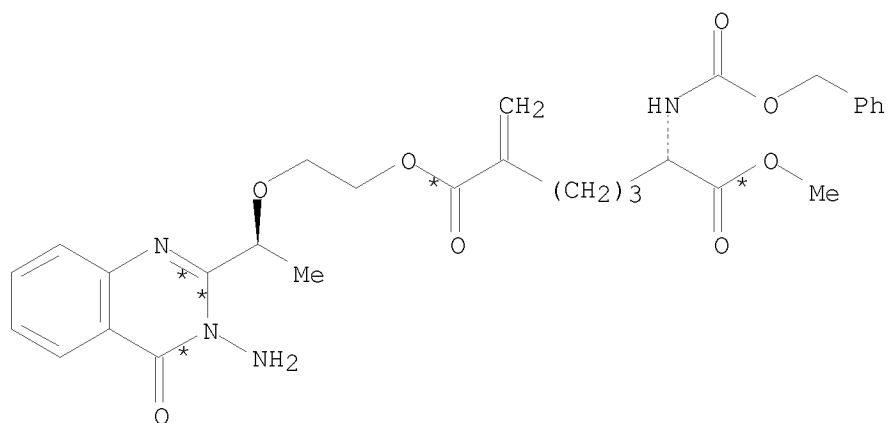


AY



BB

2  
STEPS  
→



BG

YIELD 51%

RX(15)    RCT    BA 874535-03-2, M 67-56-1  
           RGT    BC 104-15-4 TsOH  
           PRO    AF 874534-85-7, BB 874534-90-4  
           SOL    67-56-1 MeOH  
           CON    16 hours, room temperature  
           NTE    solid-supported reagent, 100% overall yield

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RX(14) RCT AY 923015-23-0

STAGE(1)

RGT AV 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 67-56-1 MeOH  
CON 19 hours, room temperature

STAGE(2)

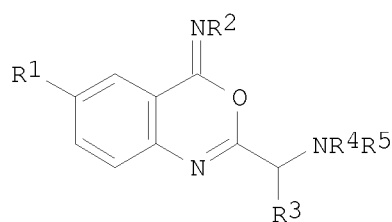
RGT AW 302-01-2 N2H4  
SOL 64-17-5 EtOH  
CON 2 hours, 140 deg C

PRO AZ 874534-89-1  
NTE sealed tube in 2nd stage

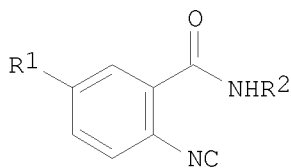
RX(18) RCT AZ 874534-89-1, BB 874534-90-4  
RGT BH 64075-39-4D Benzenemethanamine, N-(cyclohexylcarbonimidoyl)-  
PRO BG 874534-93-7  
CAT 1122-58-3 4-DMAP  
SOL 75-09-2 CH2Cl2  
CON 48 hours, room temperature  
NTE solid-supported reagent

REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 42 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 144:36301 CASREACT  
TITLE: Exploiting the Dual Reactivity of o-Isocyanobenzamide:  
Three-Component Synthesis of  
4-Imino-4H-3,1-benzoxazines  
AUTHOR(S): Bonne, Damien; Dekhane, Mouloud; Zhu, Jieping  
CORPORATE SOURCE: Institut de Chimie des Substances Naturelles, CNRS,  
Gif-sur-Yvette, 91198, Fr.  
SOURCE: Organic Letters (2005), 7(23), 5285-5288  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



I



II

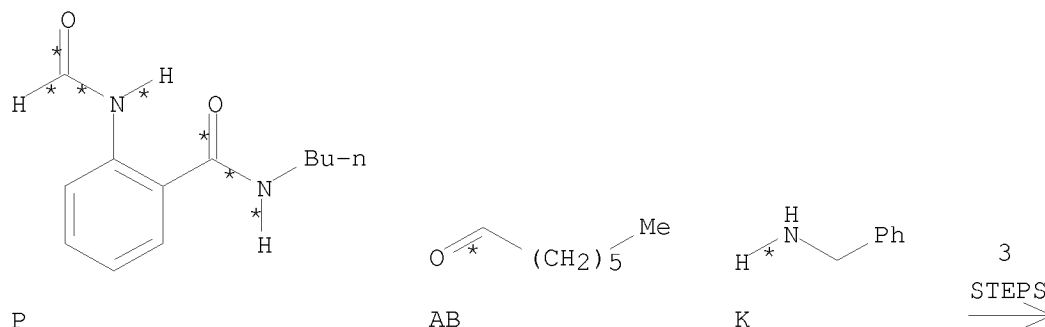
AB A multicomponent synthesis of 4-imino-4H-3,1-benzoxazines I [R1 = H, MeO;  
R2 = n-Bu, PhCH2, PhCH2CH2, (S)-PhCH2CH(CO2Me), etc.; R3 = H, Me2CH,  
cyclohexyl, n-hexyl; R4 = H, R5 = n-Bu, MeO2CCH2CH2, PhCH2,

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9-fluorenylmethyl; R4 = R5 = Me; R4R5N = morpholino] is developed.  
Heating a toluene solution of an aldehyde R3CHO, an amine R4R5NH, and an  
isonitrile II in the presence of a stoichiometric amount of ammonium  
chloride at 60 °C for 12 h produces the benzoxazines I in good to  
excellent yields.

RX(80) OF 89 COMPOSED OF RX(8), RX(19), RX(27)

RX(80) P + AB + K ==> BF



BF  
YIELD 65%

RX(8) RCT P 870672-07-4

STAGE(1)

RGT W 7087-68-5 EtN(Pr-i)2, X 10025-87-3 POC13

SOL 75-09-2 CH2Cl2

CON 2 hours, 0 deg C

STAGE(2)

RGT Y 584-08-7 K2CO3

SOL 7732-18-5 Water

PRO V 870672-10-9

RX(19) RCT AB 111-71-7, K 100-46-9

STAGE(1)

RGT AG 12125-02-9 NH4Cl

SOL 108-88-3 PhMe

CON 15 minutes, room temperature

## STAGE(2)

RCT V 870672-10-9

CON 12 hours, 60 deg C

PRO AV 870672-20-1

RX(27) RCT AV 870672-20-1  
 RGT BG 110-89-4 Piperidine  
 PRO BF 870672-28-9  
 SOL 141-78-6 AcOEt  
 CON 4 days, 70 deg C

REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 43 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 144:22759 CASREACT

TITLE: Preparation of purine quinazolinones as inhibitors of  
 human phosphatidylinositol 3-kinase delta

INVENTOR(S): Fowler, Kerry W.; Huang, Danwen; Kesicki, Edward A.;  
 Ooi, Hua Chee; Oliver, Amy R.; Ruan, Fuqiang;  
 Treiberg, Jennifer

PATENT ASSIGNEE(S): Icos Corporation, USA

SOURCE: PCT Int. Appl., 247 pp.  
 CODEN: PIXXD2

DOCUMENT TYPE: Patent

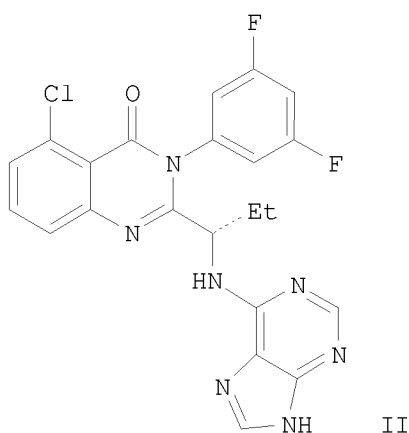
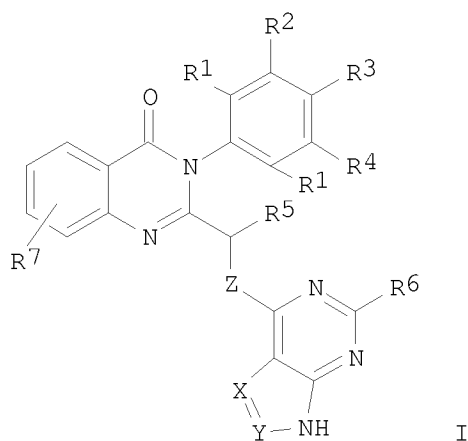
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005113556	A1	20051201	WO 2005-US16778	20050512
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2005245875	A1	20051201	AU 2005-245875	20050512
CA 2566609	A1	20051201	CA 2005-2566609	20050512
WO 2005113554	A2	20051201	WO 2005-US16661	20050512
WO 2005113554	A3	20060406		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,			

ZA, ZM, ZW  
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,  
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,  
 EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,  
 RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,  
 MR, NE, SN, TD, TG  
 EP 1761540 A1 20070314 EP 2005-752122 20050512  
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 HR, LV, MK, YU  
 CN 101031569 A 20070905 CN 2005-80023449 20050512  
 JP 2007537291 T 20071220 JP 2007-513402 20050512  
 US 20080275067 A1 20081106 US 2007-596092 20071214  
 PRIORITY APPLN. INFO.: US 2004-570784P 20040513  
 WO 2005-US16778 20050512  
 OTHER SOURCE(S): MARPAT 144:22759  
 GI

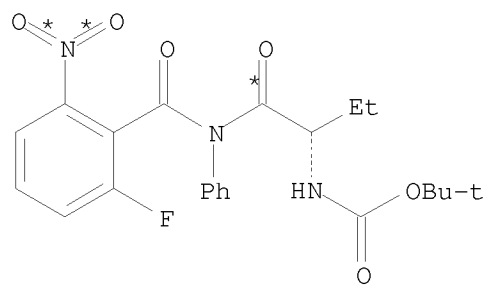


AB Quinazolinone derivs. of formula I [X, Y = N, (substituted) CH; Z = NH, O;  
 R1-R3 = H, halo, alkyl; R4 = H, halo, OH, alkoxy, CN, acyl, etc.; R5 =  
 alkyl, Ph, CH<sub>2</sub>C.tplbond.CH, etc.; R6 = H, halo, (substituted) NH<sub>2</sub>; R7 =  
 alkyl, halo, CF<sub>3</sub>, etc.; ZR5= alkylene] are prepared that inhibit  
 PI3K $\delta$  activity. Methods of inhibiting phosphatidylinositol 3-kinase  
 delta isoform (PI3K $\delta$ ) activity, and methods of treating diseases,  
 such as disorders of immunity and inflammation in which PI3K $\delta$  plays  
 a role in leukocyte function, using the compds. also are disclosed. Thus,  
 II was prepared, and had EC<sub>50</sub> value of 1.6 nM in human B lymphocyte assay.

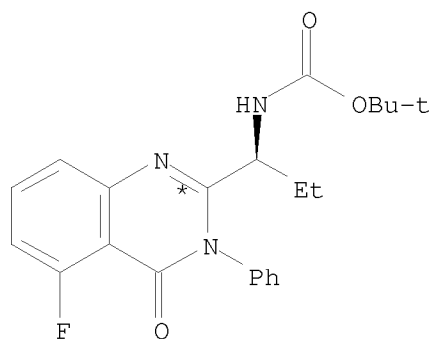
RX(110) OF 752 ...GM ==> GN...



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GM



GN

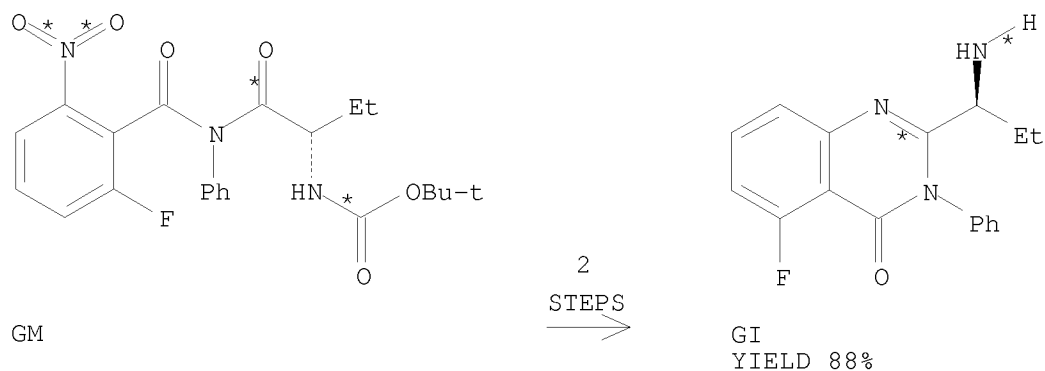
YIELD 69%

RX(110)    RCT    GM 870281-84-8  
             RGT    BO 7440-66-6 Zn  
             PRO    GN 870281-85-9  
             SOL    64-19-7 AcOH  
             CON    SUBSTAGE(1) room temperature  
                     SUBSTAGE(2) <35 deg C  
                     SUBSTAGE(3) <35 deg C  
                     SUBSTAGE(4) <35 deg C -> room temperature  
                     SUBSTAGE(5) 2 hours, room temperature

RX(233) OF 752 COMPOSED OF RX(110), RX(111)

RX(233)    GM    ==>    GI

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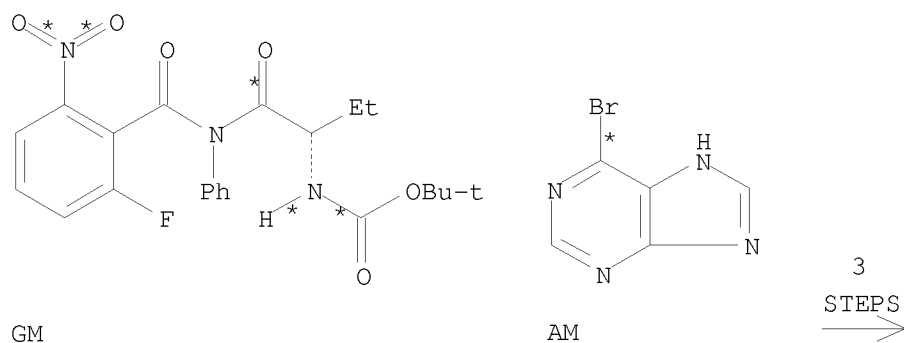
RX(110) RCT GM 870281-84-8  
RGT BO 7440-66-6 Zn  
PRO GN 870281-85-9  
SOL 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) <35 deg C  
SUBSTAGE(3) <35 deg C  
SUBSTAGE(4) <35 deg C -> room temperature  
SUBSTAGE(5) 2 hours, room temperature

RX(111) RCT GN 870281-85-9  
STAGE(1)  
RGT BJ 76-05-1 F3CCO2H  
SOL 75-09-2 CH2Cl2  
CON 1 hour, room temperature

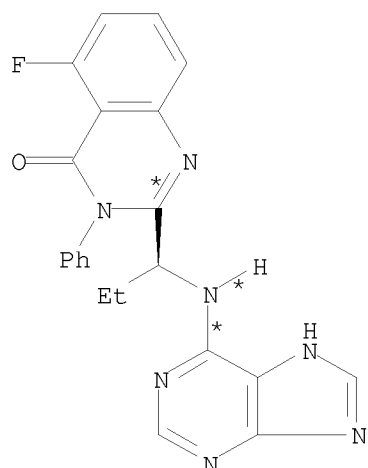
STAGE(2)  
RGT W 584-08-7 K2CO3  
SOL 7732-18-5 Water, 75-09-2 CH2Cl2  
CON room temperature, pH >10

PRO GI 870281-86-0

RX(357) OF 752 COMPOSED OF RX(110), RX(111), RX(107)  
RX(357) GM + AM ==> GJ



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GJ  
YIELD 50%

RX(110) RCT GM 870281-84-8  
RGT BO 7440-66-6 Zn  
PRO GN 870281-85-9  
SOL 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) <35 deg C  
SUBSTAGE(3) <35 deg C  
SUBSTAGE(4) <35 deg C -> room temperature  
SUBSTAGE(5) 2 hours, room temperature

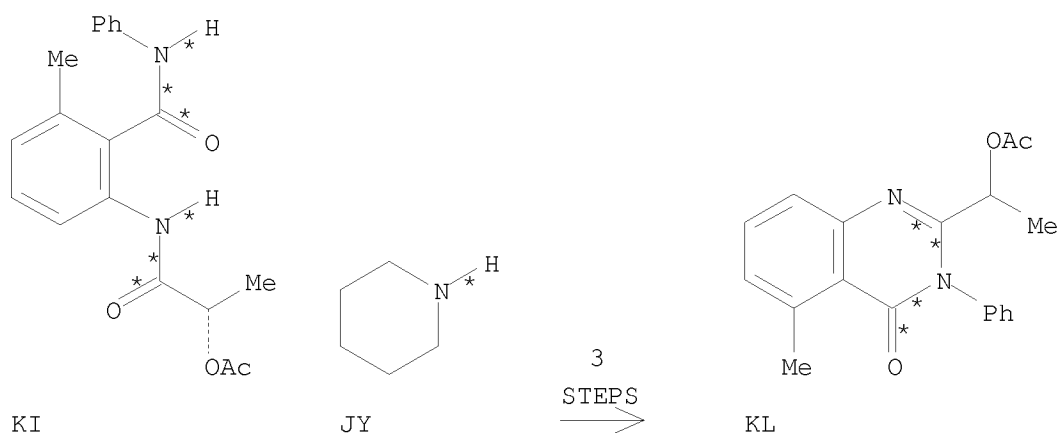
RX(111) RCT GN 870281-85-9  
  
STAGE(1)  
RGT BJ 76-05-1 F3CCO2H  
SOL 75-09-2 CH2Cl2  
CON 1 hour, room temperature

STAGE(2)  
RGT W 584-08-7 K2CO3  
SOL 7732-18-5 Water, 75-09-2 CH2Cl2  
CON room temperature, pH >10

PRO GI 870281-86-0

RX(107) RCT GI 870281-86-0, AM 767-69-1  
RGT AE 7087-68-5 EtN(Pr-i)2  
PRO GJ 870281-82-6  
SOL 75-65-0 t-BuOH  
CON SUBSTAGE(1) room temperature -> 80 deg C  
SUBSTAGE(2) 24 hours, 80 deg C

RX(448) OF 752 COMPOSED OF RX(174), RX(175), RX(176)  
RX(448) KI + JY ==> KL



RX(174) RCT KI 870282-48-7

STAGE(1)

RGT AE 7087-68-5 EtN(Pr-i)2, JX 7553-56-2 I2, IO 603-35-0 PPh3  
 SOL 75-09-2 CH2Cl2  
 CON 4 days, room temperature

STAGE(2)

RGT BM 144-55-8 NaHCO3  
 SOL 7732-18-5 Water  
 CON room temperature

PRO KJ 870282-49-8

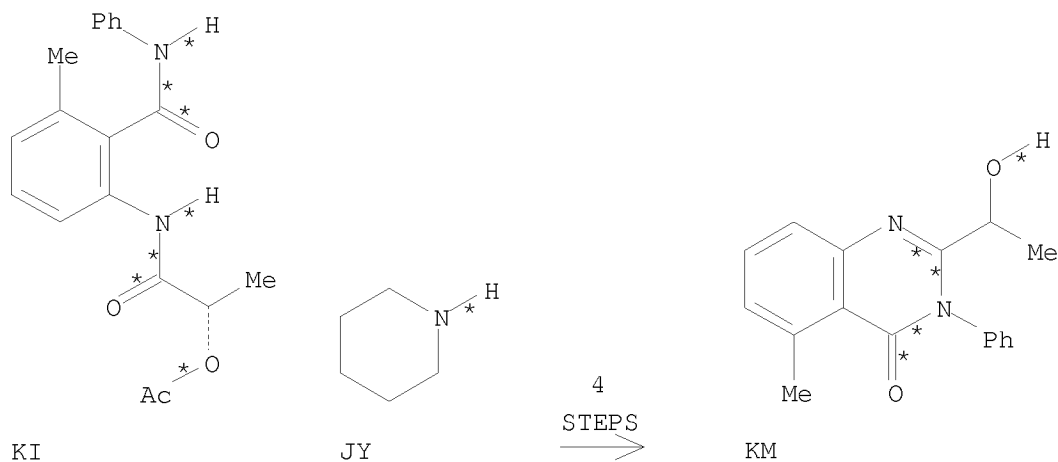
RX(175) RCT KJ 870282-49-8, JY 110-89-4  
 PRO KK 870282-50-1  
 CON 19.5 hours, room temperature  
 NTE other product also detected

RX(176) RCT KK 870282-50-1  
 PRO KL 870282-51-2  
 SOL 75-05-8 MeCN  
 CON SUBSTAGE(1) room temperature -> reflux  
 SUBSTAGE(2) 3 hours, reflux

RX(451) OF 752 COMPOSED OF RX(174), RX(175), RX(176), RX(177)

RX(451) KI + JY ==> KM

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RX(174) RCT KI 870282-48-7

STAGE(1)

RGT AE 7087-68-5 EtN(Pr-i)2, JX 7553-56-2 I2, IO 603-35-0 PPh3  
SOL 75-09-2 CH2Cl2  
CON 4 days, room temperature

STAGE(2)

RGT BM 144-55-8 NaHCO3  
SOL 7732-18-5 Water  
CON room temperature

PRO KJ 870282-49-8

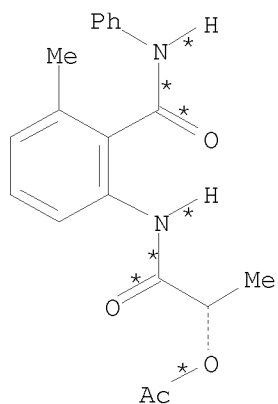
RX(175) RCT KJ 870282-49-8, JY 110-89-4  
PRO KK 870282-50-1  
CON 19.5 hours, room temperature  
NTE other product also detected

RX(176) RCT KK 870282-50-1  
PRO KL 870282-51-2  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) room temperature -> reflux  
SUBSTAGE(2) 3 hours, reflux

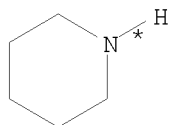
RX(177) RCT KL 870282-51-2  
RGT W 584-08-7 K2CO3  
PRO KM 870282-52-3  
SOL 67-56-1 MeOH  
CON 20 minutes, room temperature

RX(723) OF 752 COMPOSED OF RX(174), RX(175), RX(176), RX(177), RX(178)  
RX(723) KI + JY + AV ==> KF

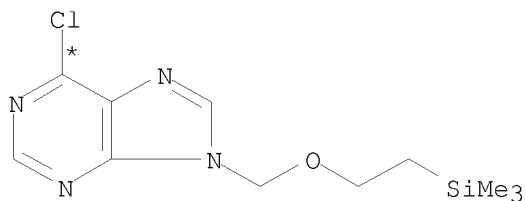
10/ 562,112



KI

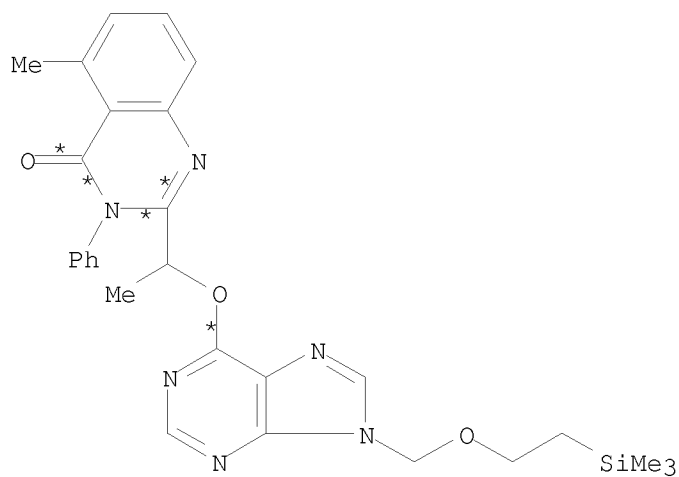


JY



AV

5  
STEPS  
→



KF

RX(174) RCT KI 870282-48-7

STAGE(1)

RGT AE 7087-68-5 EtN(Pr-i)<sub>2</sub>, JX 7553-56-2 I<sub>2</sub>, IO 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON 4 days, room temperature

STAGE(2)

RGT BM 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water

CON room temperature

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PRO KJ 870282-49-8

RX(175) RCT KJ 870282-49-8, JY 110-89-4  
PRO KK 870282-50-1  
CON 19.5 hours, room temperature  
NTE other product also detected

RX(176) RCT KK 870282-50-1  
PRO KL 870282-51-2  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) room temperature -> reflux  
SUBSTAGE(2) 3 hours, reflux

RX(177) RCT KL 870282-51-2  
RGT W 584-08-7 K2CO3  
PRO KM 870282-52-3  
SOL 67-56-1 MeOH  
CON 20 minutes, room temperature

RX(178) RCT KM 870282-52-3

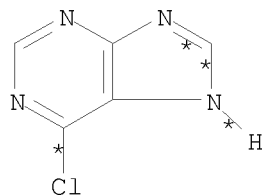
STAGE(1)  
RGT KN 7646-69-7 NaH  
SOL 109-99-9 THF  
CON 10 minutes, room temperature

STAGE(2)  
RCT AV 222296-31-3  
SOL 109-99-9 THF  
CON SUBSTAGE(1) 21.5 hours, room temperature  
SUBSTAGE(2) 1.5 hours, room temperature  
SUBSTAGE(3) 1 hour, room temperature

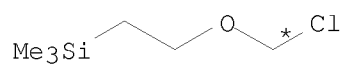
STAGE(3)  
RGT KO 12125-02-9 NH4Cl  
SOL 7732-18-5 Water  
CON room temperature

PRO KF 870282-53-4

RX(727) OF 752 COMPOSED OF REACTION SEQUENCE RX(13), RX(178)  
AND REACTION SEQUENCE RX(174), RX(175), RX(176), RX(177),  
RX(178)  
...AU + AN ==> AV...  
... KI + JY + AV ==> KF



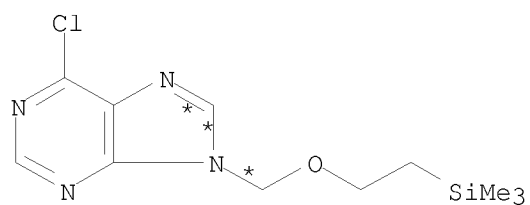
AU



AN

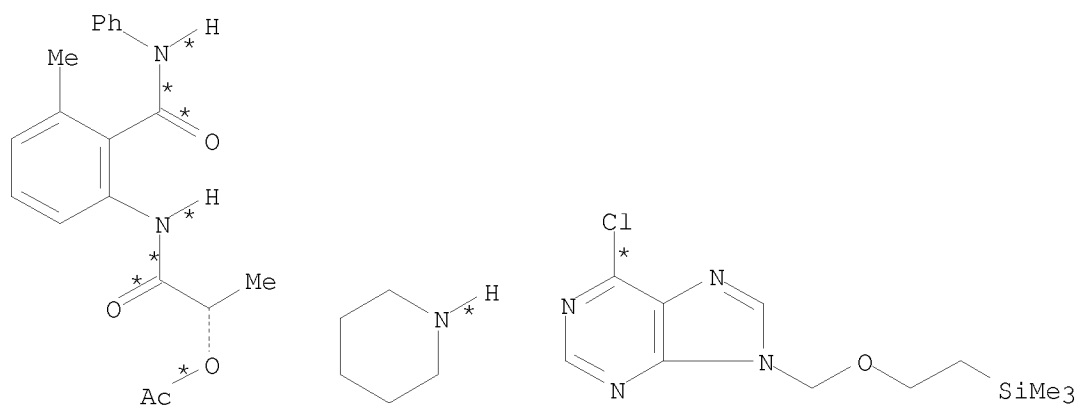
5  
STEPS  
→

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AV

START NEXT REACTION SEQUENCE

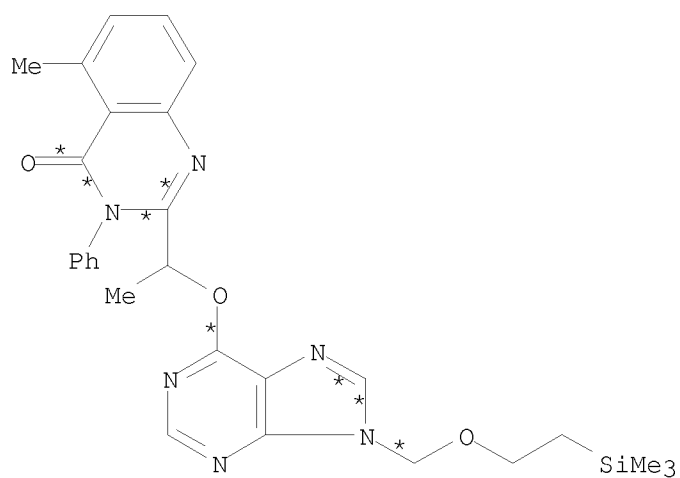


KI

JY

AV

5  
STEPS  
→



KF

RX(13)    RCT    AU 87-42-3, AN 76513-69-4  
          RGT    W 584-08-7 K2CO3  
          PRO    AV 222296-31-3  
          SOL    68-12-2 DMF  
          CON    18 hours, room temperature



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NTE mol. sieves used

RX(174) RCT KI 870282-48-7

STAGE(1)

RGT AE 7087-68-5 EtN(Pr-i)<sub>2</sub>, JX 7553-56-2 I<sub>2</sub>, IO 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON 4 days, room temperature

STAGE(2)

RGT BM 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water

CON room temperature

PRO KJ 870282-49-8

RX(175) RCT KJ 870282-49-8, JY 110-89-4

PRO KK 870282-50-1

CON 19.5 hours, room temperature

NTE other product also detected

RX(176) RCT KK 870282-50-1

PRO KL 870282-51-2

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 3 hours, reflux

RX(177) RCT KL 870282-51-2

RGT W 584-08-7 K<sub>2</sub>CO<sub>3</sub>

PRO KM 870282-52-3

SOL 67-56-1 MeOH

CON 20 minutes, room temperature

RX(178) RCT KM 870282-52-3

STAGE(1)

RGT KN 7646-69-7 NaH

SOL 109-99-9 THF

CON 10 minutes, room temperature

STAGE(2)

RCT AV 222296-31-3

SOL 109-99-9 THF

CON SUBSTAGE(1) 21.5 hours, room temperature

SUBSTAGE(2) 1.5 hours, room temperature

SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RGT KO 12125-02-9 NH<sub>4</sub>Cl

SOL 7732-18-5 Water

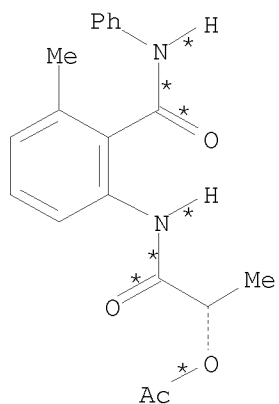
CON room temperature

PRO KF 870282-53-4

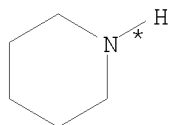
RX(728) OF 752 COMPOSED OF RX(174), RX(175), RX(176), RX(177), RX(178), RX(172)

RX(728) KI + JY + AV ==> KG

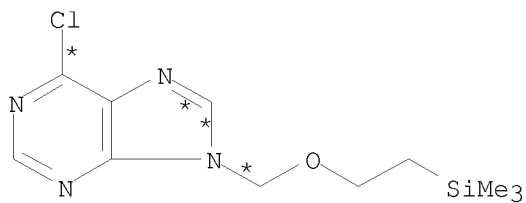
10/ 562,112



KI

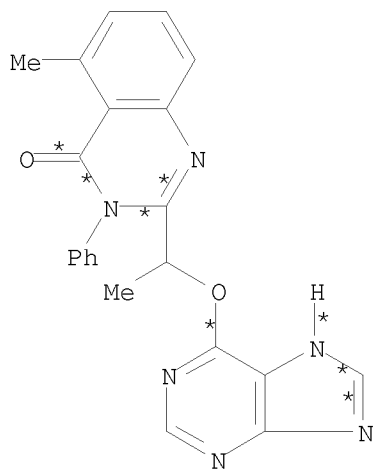


JY



AV

6  
STEPS  
→



KG

RX(174) RCT KI 870282-48-7

STAGE(1)

RGT AE 7087-68-5 EtN(Pr-i)2, JX 7553-56-2 I2, IO 603-35-0 PPh3  
SOL 75-09-2 CH2Cl2  
CON 4 days, room temperature

STAGE(2)

RGT BM 144-55-8 NaHCO3  
SOL 7732-18-5 Water  
CON room temperature

PRO KJ 870282-49-8

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RX(175) RCT KJ 870282-49-8, JY 110-89-4  
PRO KK 870282-50-1  
CON 19.5 hours, room temperature  
NTE other product also detected

RX(176) RCT KK 870282-50-1  
PRO KL 870282-51-2  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) room temperature -> reflux  
SUBSTAGE(2) 3 hours, reflux

RX(177) RCT KL 870282-51-2  
RGT W 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO KM 870282-52-3  
SOL 67-56-1 MeOH  
CON 20 minutes, room temperature

RX(178) RCT KM 870282-52-3

STAGE(1)

RGT KN 7646-69-7 NaH  
SOL 109-99-9 THF  
CON 10 minutes, room temperature

STAGE(2)

RCT AV 222296-31-3  
SOL 109-99-9 THF  
CON SUBSTAGE(1) 21.5 hours, room temperature  
SUBSTAGE(2) 1.5 hours, room temperature  
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RGT KO 12125-02-9 NH<sub>4</sub>Cl  
SOL 7732-18-5 Water  
CON room temperature

PRO KF 870282-53-4

RX(172) RCT KF 870282-53-4

STAGE(1)

RGT AH 7647-01-0 HCl  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON SUBSTAGE(1) room temperature -> 40 deg C  
SUBSTAGE(2) 3 hours, 40 deg C  
SUBSTAGE(3) cooled

STAGE(2)

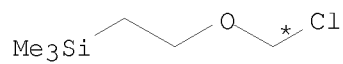
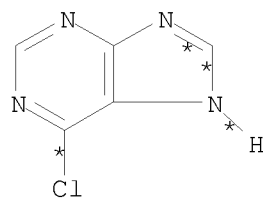
RGT W 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
SOL 7732-18-5 Water  
CON room temperature, pH 10

PRO KG 870282-47-6

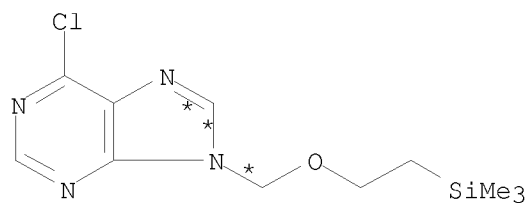
RX(734) OF 752 COMPOSED OF REACTION SEQUENCE RX(13), RX(178), RX(172)  
AND REACTION SEQUENCE RX(174), RX(175), RX(176), RX(177),  
RX(178), RX(172)  
...AU + AN ==> AV...

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... KI + JY + AV ==> KG

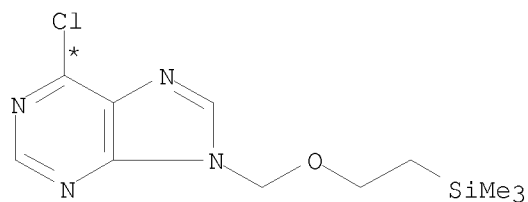
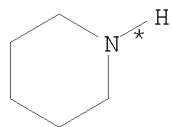
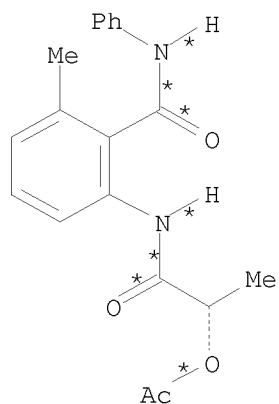


6  
STEPS  
→



AV

START NEXT REACTION SEQUENCE

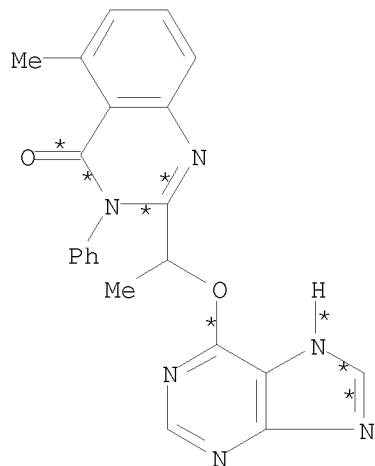


KI

JY

AV

6  
STEPS  
→



KG

RX(13) RCT AU 87-42-3, AN 76513-69-4  
 RGT W 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO AV 222296-31-3  
 SOL 68-12-2 DMF  
 CON 18 hours, room temperature  
 NTE mol. sieves used

RX(174) RCT KI 870282-48-7

## STAGE(1)

RGT AE 7087-68-5 EtN(Pr-i)<sub>2</sub>, JX 7553-56-2 I<sub>2</sub>, IO 603-35-0 PPh<sub>3</sub>  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON 4 days, room temperature

## STAGE(2)

RGT BM 144-55-8 NaHCO<sub>3</sub>  
 SOL 7732-18-5 Water  
 CON room temperature

PRO KJ 870282-49-8

RX(175) RCT KJ 870282-49-8, JY 110-89-4  
 PRO KK 870282-50-1  
 CON 19.5 hours, room temperature  
 NTE other product also detected

RX(176) RCT KK 870282-50-1  
 PRO KL 870282-51-2  
 SOL 75-05-8 MeCN  
 CON SUBSTAGE(1) room temperature -> reflux  
 SUBSTAGE(2) 3 hours, reflux

RX(177) RCT KL 870282-51-2  
 RGT W 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO KM 870282-52-3  
 SOL 67-56-1 MeOH  
 CON 20 minutes, room temperature

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RX(178) RCT KM 870282-52-3

STAGE(1)

RGT KN 7646-69-7 NaH  
SOL 109-99-9 THF  
CON 10 minutes, room temperature

STAGE(2)

RCT AV 222296-31-3  
SOL 109-99-9 THF  
CON SUBSTAGE(1) 21.5 hours, room temperature  
SUBSTAGE(2) 1.5 hours, room temperature  
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RGT KO 12125-02-9 NH4Cl  
SOL 7732-18-5 Water  
CON room temperature

PRO KF 870282-53-4

RX(172) RCT KF 870282-53-4

STAGE(1)

RGT AH 7647-01-0 HCl  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON SUBSTAGE(1) room temperature -> 40 deg C  
SUBSTAGE(2) 3 hours, 40 deg C  
SUBSTAGE(3) cooled

STAGE(2)

RGT W 584-08-7 K2CO3  
SOL 7732-18-5 Water  
CON room temperature, pH 10

PRO KG 870282-47-6

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 44 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 143:460174 CASREACT

TITLE: Preparation of heterocyclic amides as MMP-13  
inhibitors for treating osteoarthritis and rheumatoid  
arthritis

INVENTOR(S): Terauchi, Jun; Kuno, Haruhiko; Nara, Hiroshi; Oki,  
Hideyuki; Sato, Kenjiro

PATENT ASSIGNEE(S): Takeda Pharmaceutical Company Limited, Japan

SOURCE: PCT Int. Appl., 455 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

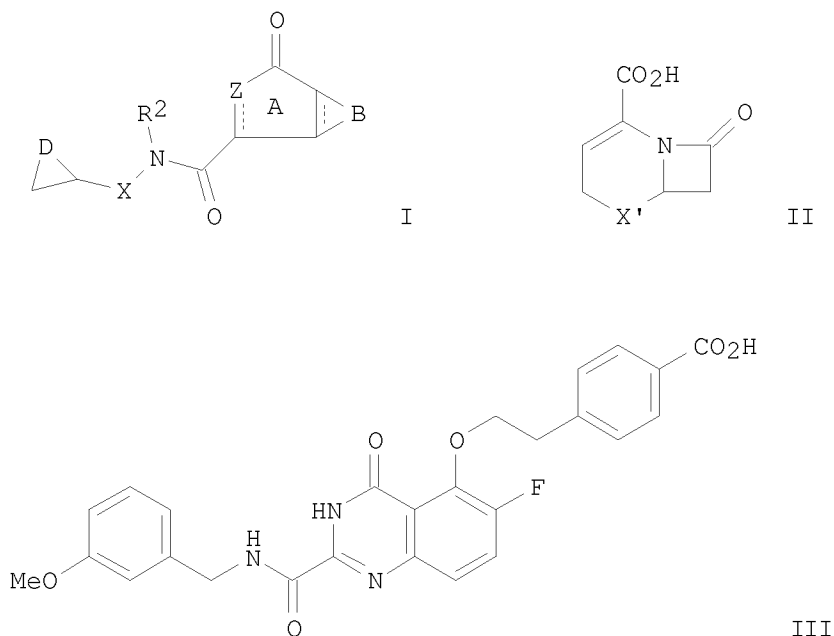
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

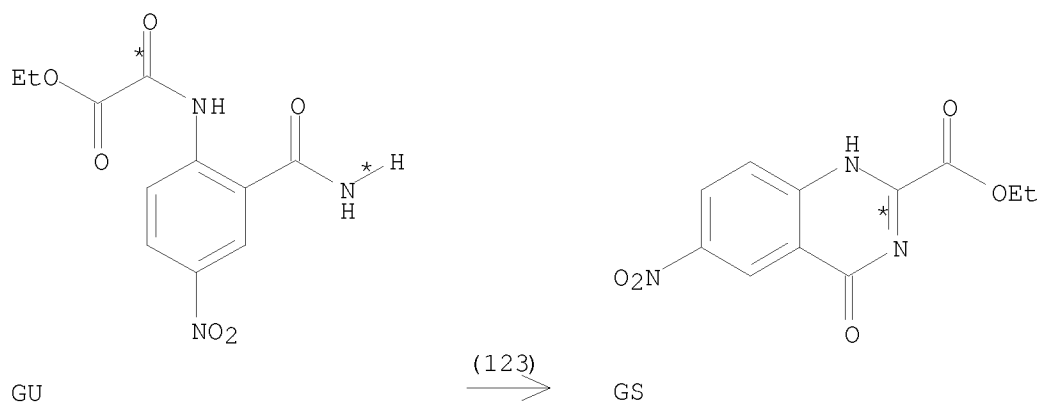
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2005238386	A1	20051110	AU 2005-238386	20050428
CA 2564085	A1	20051110	CA 2005-2564085	20050428
EP 1740551	A1	20070110	EP 2005-739012	20050428
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU			
CN 1976907	A	20070606	CN 2005-80021727	20050428
BR 2005010305	A	20071002	BR 2005-10305	20050428
JP 2007535488	T	20071206	JP 2006-540833	20050428
MX 2006012333	A	20070117	MX 2006-12333	20061025
US 20080027050	A1	20080131	US 2006-579298	20061030
IN 2006KN03427	A	20070615	IN 2006-KN3427	20061120
KR 2007008709	A	20070117	KR 2006-724701	20061124
NO 2006005537	A	20070129	NO 2006-5537	20061130
PRIORITY APPLN. INFO.:			JP 2004-135596	20040430
			WO 2005-JP8549	20050428
OTHER SOURCE(S):	MARPAT 143:460174			
GI				



AB The invention is related to the preparation of heterocyclic amides of formula I [A = (un)substituted N-containing heterocycle; B = (un)substituted monocyclic homocycle or heterocycle; Z = N, NH and derivs.; R2 = H, (un)substituted hydrocarbyl; X = (un)substituted spacer; D = (un)substituted heterocycle other than II; X' = S, O, SO, CH2; and at least one of B and C has substituent(s); with the exception of 2 compds.; their salts, and their prodrugs] having a matrix metalloproteinase, particularly MMP-13, inhibitory activity. Thus, reacting 5,6-difluoro-N-[[3-(methyloxy)phenyl]methyl]-4-oxo-3,4-dihydroquinazoline-2-carboxamide (preparation given) with 4-(2-hydroxyethyl)benzoic acid gave amide III in 70% yield. III displayed an inhibitory rate of 99% towards MMP-13 activity. I are useful for treating osteoarthritis and rheumatoid arthritis.

RX(123) OF 1000 GU ==> GS...



RX(123) RCT GU 54166-78-8

STAGE(1)

RGT FB 141-52-6 NaOEt  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 0 deg C -> room temperature  
SUBSTAGE(3) 12 hours, room temperature

STAGE(2)

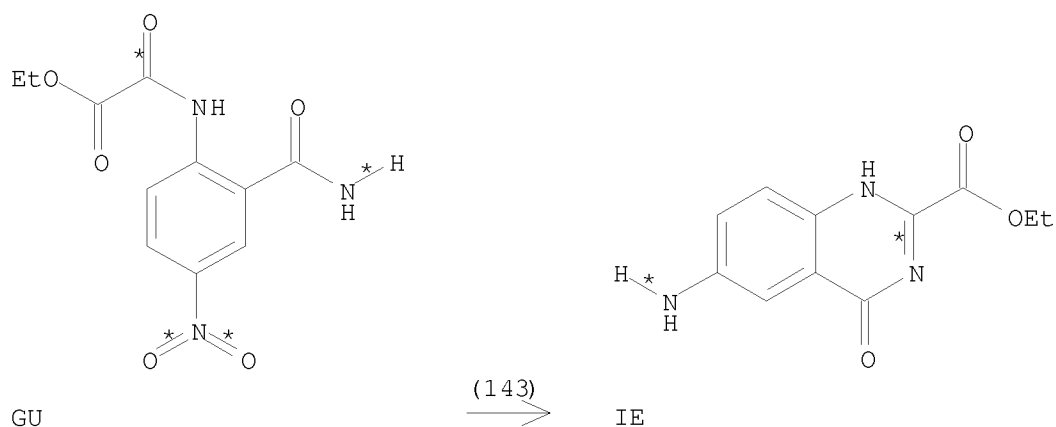
RGT GV 77-92-9 Citric acid  
SOL 7732-18-5 Water  
CON room temperature

PRO GS 34632-65-0

RX(143) OF 1000 GU ==> IE...



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RX(143) RCT GU 54166-78-8

STAGE(1)

RGT CI 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 64-17-5 EtOH, 109-99-9 THF  
CON 8 hours, room temperature

STAGE(2)

RGT FB 141-52-6 NaOEt  
SOL 64-17-5 EtOH, 109-99-9 THF  
CON 12 hours, room temperature

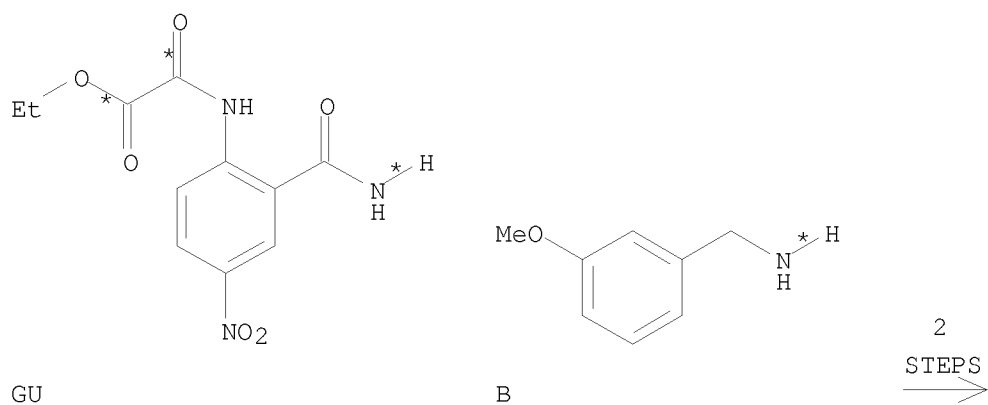
STAGE(3)

RGT GV 77-92-9 Citric acid  
SOL 7732-18-5 Water  
CON room temperature

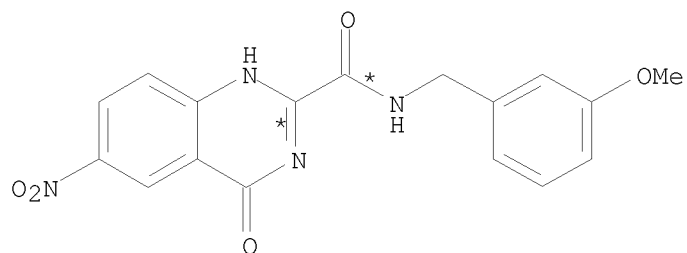
PRO IE 34632-66-1

RX(725) OF 1000 COMPOSED OF RX(123), RX(122)

RX(725) GU + B ==> GT



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GT

RX(123) RCT GU 54166-78-8

STAGE(1)

RGT FB 141-52-6 NaOEt

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 0 deg C -> room temperature

SUBSTAGE(3) 12 hours, room temperature

STAGE(2)

RGT GV 77-92-9 Citric acid

SOL 7732-18-5 Water

CON room temperature

PRO GS 34632-65-0

RX(122) RCT B 5071-96-5, GS 34632-65-0

RGT D 121-44-8 Et<sub>3</sub>N

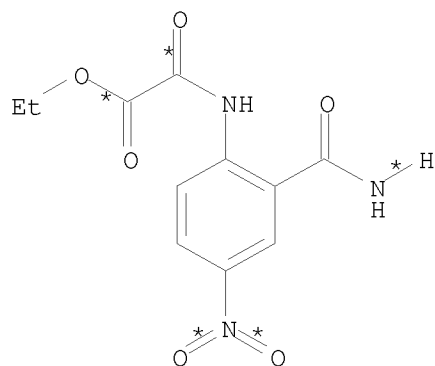
PRO GT 869294-63-3

SOL 109-99-9 THF

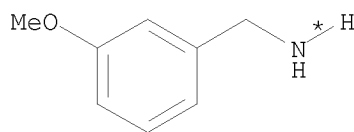
CON overnight, room temperature

RX(740) OF 1000 COMPOSED OF RX(143), RX(144)

RX(740) GU + B ==> IF



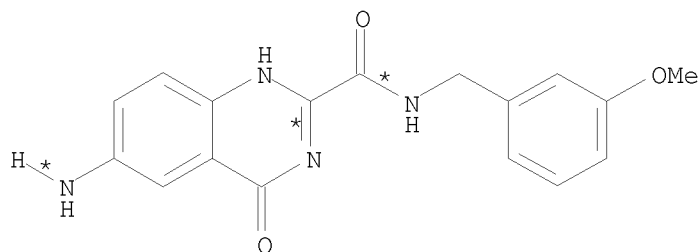
GU



B

2  
STEPS  
→

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IF

RX(143) RCT GU 54166-78-8

STAGE(1)

RGT CI 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 64-17-5 EtOH, 109-99-9 THF  
CON 8 hours, room temperature

STAGE(2)

RGT FB 141-52-6 NaOEt  
SOL 64-17-5 EtOH, 109-99-9 THF  
CON 12 hours, room temperature

STAGE(3)

RGT GV 77-92-9 Citric acid  
SOL 7732-18-5 Water  
CON room temperature

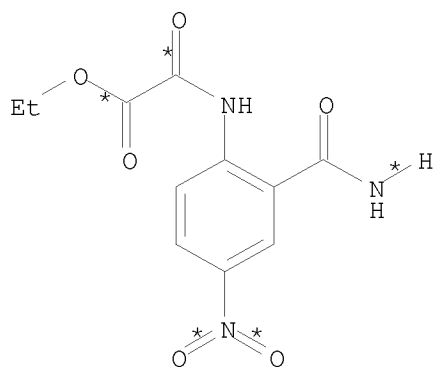
PRO IE 34632-66-1

RX(144) RCT B 5071-96-5, IE 34632-66-1  
RGT D 121-44-8 Et3N  
PRO IF 869294-81-5  
SOL 109-99-9 THF  
CON overnight, room temperature

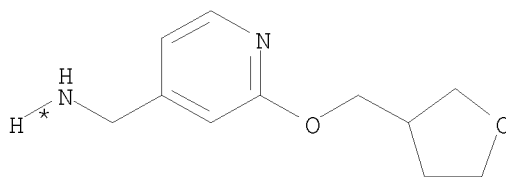
RX(741) OF 1000 COMPOSED OF RX(143), RX(145)

RX(741) GU + AD ==> IG

10/ 562,112

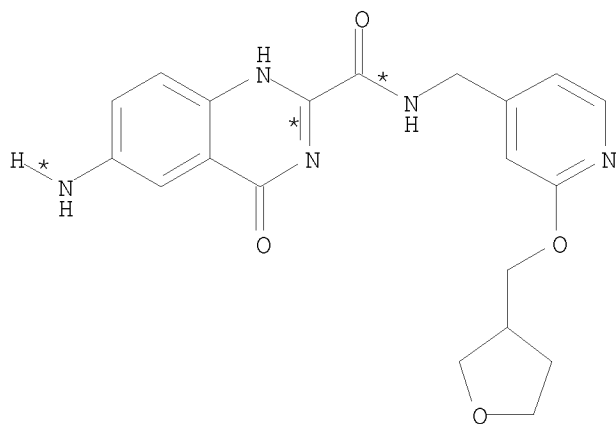


GU



AD

2  
STEPS  
→



IG

RX(143) RCT GU 54166-78-8

STAGE(1)

RGT CI 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 64-17-5 EtOH, 109-99-9 THF  
CON 8 hours, room temperature

STAGE(2)

RGT FB 141-52-6 NaOEt  
SOL 64-17-5 EtOH, 109-99-9 THF  
CON 12 hours, room temperature

STAGE(3)

RGT GV 77-92-9 Citric acid  
SOL 7732-18-5 Water  
CON room temperature

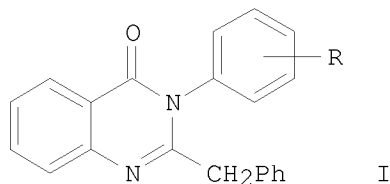
PRO IE 34632-66-1

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RX(145) RCT AD 869293-60-7, IE 34632-66-1  
RGT D 121-44-8 Et3N  
PRO IG 869294-82-6  
SOL 109-99-9 THF  
CON overnight, room temperature

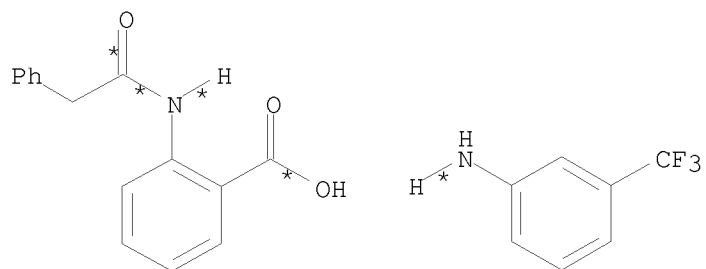
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 45 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 143:367264 CASREACT  
TITLE: Green chemical multicomponent one-pot synthesis of  
fluorinated 2,3-disubstituted quinazolin-4(3H)-ones  
under solvent-free conditions and their antifungal  
activity  
AUTHOR(S): Dandia, Anshu; Singh, Ruby; Sarawgi, Pritima  
CORPORATE SOURCE: Department of Chemistry, University of Rajasthan,  
Jaipur, 302004, India  
SOURCE: Journal of Fluorine Chemistry (2005), 126(3), 307-312  
CODEN: JFLCAR; ISSN: 0022-1139  
PUBLISHER: Elsevier B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB A rapid one-pot solvent-free procedure has been developed for the  
synthesis of fluorinated 2,3-disubstituted quinazolin-4(3H)-ones, e.g., I  
(R = 2-F, 3-F, 4-F, 2-CF<sub>3</sub>, 3-CF<sub>3</sub>), by neat three-component  
cyclocondensation of anthranilic acid, phenylacetyl chloride and  
substituted anilines under microwave irradiation. The exptl. methodol. and  
microwave conditions described here are well established, allowing  
significant rate enhancement and good yields compared to conventional  
reaction conditions. The reaction is generalized for o-, m- and  
p-substituted anilines with electron-donating and -withdrawing groups to  
give quinazolin-4(3H)-ones. The synthesized compds. have been screened  
for their antifungal activity.

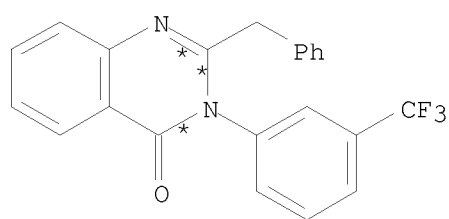
RX(1) OF 11 A + B ==> C



A

B

(1)  $\longrightarrow$



C

YIELD 88%

RX(1) RCT A 28565-98-2

STAGE(1)

RGT D 1318-93-0 Montmorillonite, E 108-24-7 Ac2O

CON 3 minutes, 141 deg C

STAGE(2)

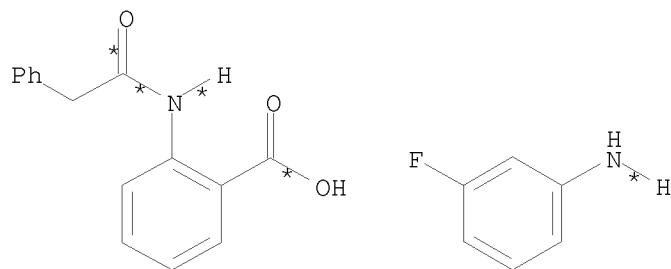
RCT B 98-16-8

CON 7 minutes, 141 deg C

PRO C 848085-19-8

NTE green chemistry, green chemistry-process simplification,  
microwave irradiation, no solvent, solid-supported reagent

RX(2) OF 11 A + F  $\implies$  G

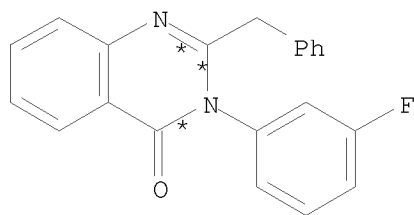


A

F

(2)  $\longrightarrow$

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G  
YIELD 82%

RX(2) RCT A 28565-98-2

STAGE(1)

RGT D 1318-93-0 Montmorillonite, E 108-24-7 Ac2O  
CON 3 minutes, 142 deg C

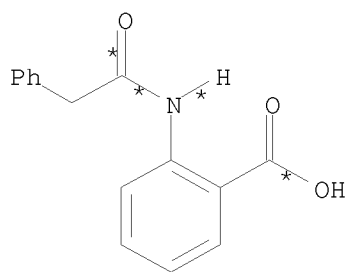
STAGE(2)

RCT F 372-19-0  
CON 6 minutes, 142 deg C

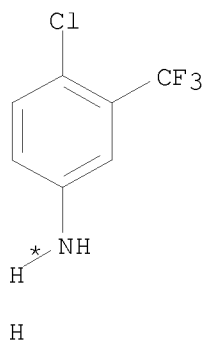
PRO G 848085-20-1

NTE green chemistry, green chemistry-process simplification,  
microwave irradiation, no solvent, solid-supported reagent

RX(3) OF 11 A + H ==> I



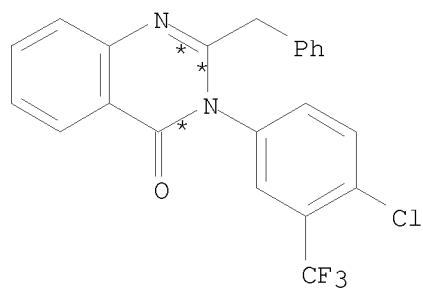
A



H

(3) >

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I  
YIELD 81%

RX(3) RCT A 28565-98-2

STAGE(1)

RGT D 1318-93-0 Montmorillonite, E 108-24-7 Ac<sub>2</sub>O  
CON 3 minutes, 137 deg C

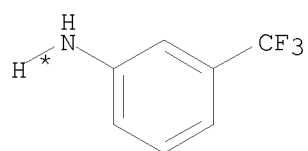
STAGE(2)

RCT H 320-51-4  
CON 7 minutes, 137 deg C

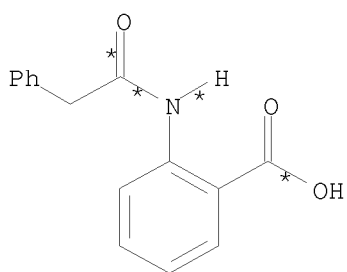
PRO I 848085-21-2

NTE green chemistry, green chemistry-process simplification,  
microwave irradiation, no solvent, solid-supported reagent

RX(10) OF 11 B + A ==> C



B

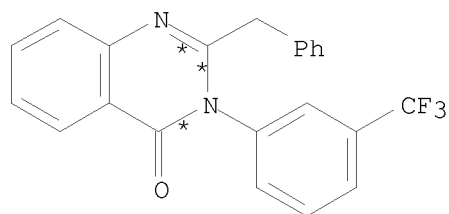


A

(10)  
→



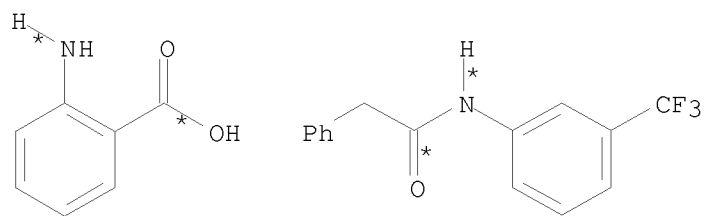
10/ 562,112



C  
YIELD 91%

RX(10)     RCT   B 98-16-8, A 28565-98-2  
             PRO   C 848085-19-8  
             CON   4 minutes, 162 deg C  
             NTE   green chemistry, green chemistry-process simplification,  
                     microwave irradiation, no solvent

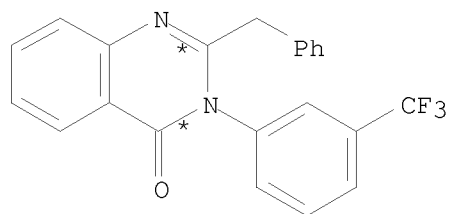
RX(11) OF 11     J   +   R   ==>   C



J

R

(11)

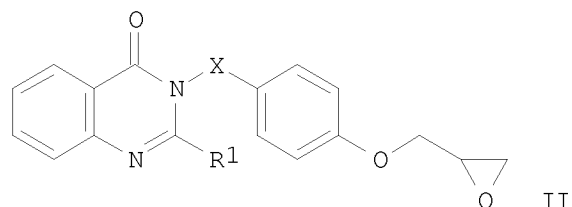
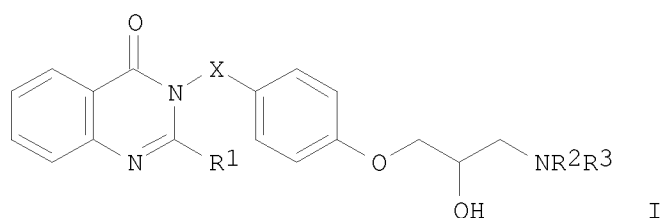


C  
YIELD 90%

RX(11)     RCT   J 118-92-3, R 1939-21-5  
             PRO   C 848085-19-8  
             CON   5 minutes, 164 deg C  
             NTE   green chemistry, green chemistry-process simplification,  
                     microwave irradiation, no solvent

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

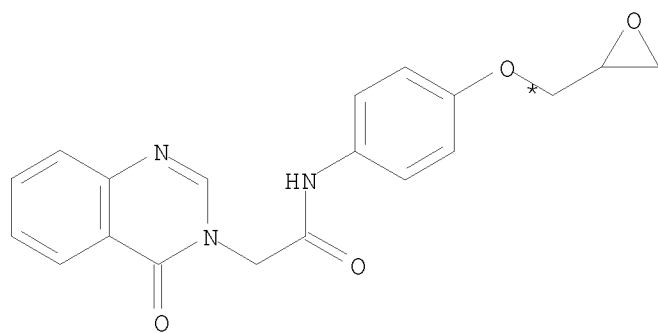
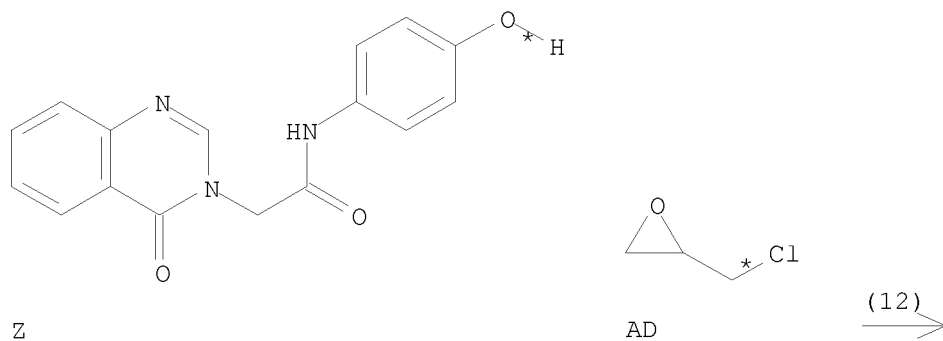
L3 ANSWER 46 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 143:286363 CASREACT  
 TITLE: Synthesis of certain (heterocyclic substituted aryloxy) propanolamines as potential adrenoceptor antagonists  
 AUTHOR(S): Khalil, N. A.; Botros, S.; Soliman, L. N.; Amin, F. M.; El-Zanfaly, S.  
 CORPORATE SOURCE: Organic Chemistry Department, Faculty of Pharmacy, Cairo University, Cairo, Egypt  
 SOURCE: Bulletin of the Faculty of Pharmacy (Cairo University) (2002), 40(1), 23-29  
 CODEN: BFPHA8; ISSN: 1110-0931  
 PUBLISHER: Cairo University, Faculty of Pharmacy  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Amino(hydroxy)-functionalized quinazolinones I [X = nothing, CH<sub>2</sub>CONH; R<sub>1</sub> = H, Me; R<sub>2</sub> = H, R<sub>3</sub> = n-Pr, Me<sub>2</sub>CH, Me<sub>3</sub>C, cyclohexyl, PhCH<sub>2</sub>, PhCH<sub>2</sub>CH<sub>2</sub>; R<sub>2</sub> = R<sub>3</sub> = Et, PhCH<sub>2</sub>; R<sub>2</sub>R<sub>3</sub>N = 1-pyrrolidinyl, 4-morpholinyl, 1-piperidinyl, 4-(4-methoxyphenyl)-1-piperazinyl, etc.] were prepared by ring opening of epoxides II with the corresponding primary and secondary amines. Pharmacol. screening showed that I (X = nothing; R<sub>1</sub> = Me; R<sub>2</sub> = H; R<sub>3</sub> = n-Bu, PhCH<sub>2</sub>CH<sub>2</sub>), I (X = CH<sub>2</sub>CONH; R<sub>1</sub> = H; R<sub>2</sub> = R<sub>3</sub> = Et; R<sub>2</sub> = H, R<sub>3</sub> = PhCH<sub>2</sub>) and I (X = CH<sub>2</sub>CONH; R<sub>1</sub> = Me; R<sub>2</sub> = H; R<sub>3</sub> = Me<sub>2</sub>CH) exhibited  $\beta$ -adrenergic blocking activity and antagonized the stimulant effect of isoprenaline on isolated frog heart.

RX(12) OF 57 ...Z + AD ==> AE...

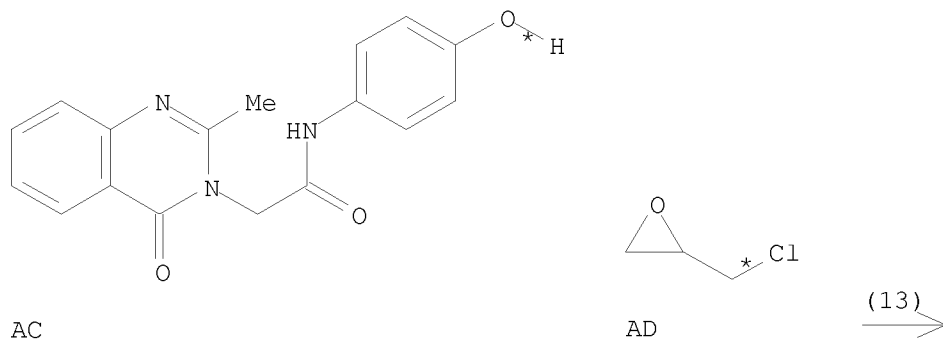
10/ 562,112



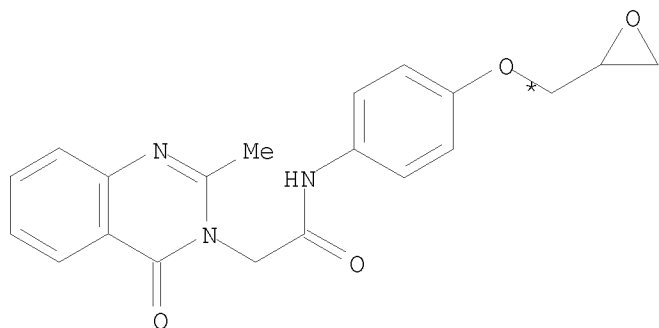
AE  
YIELD 92%

RX(12)      RCT    Z 591213-29-5, AD 106-89-8  
               RGT    AF 1310-58-3 KOH  
               PRO    AE 864234-49-1  
               SOL    7732-18-5 Water  
               CON    overnight, room temperature

RX(13) OF 57      ...AC + AD ==> AH...



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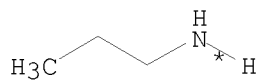


AH

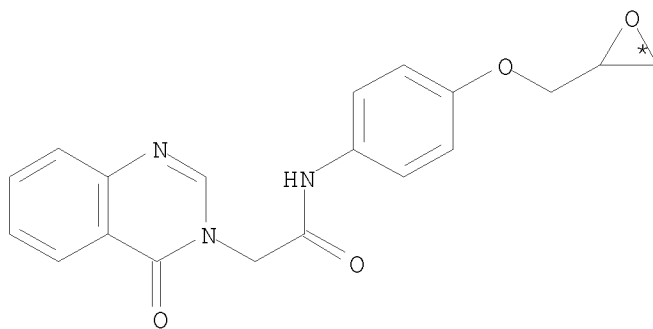
YIELD 78%

RX(13) RCT AC 864234-48-0, AD 106-89-8  
RGT AF 1310-58-3 KOH  
PRO AH 864234-50-4  
SOL 7732-18-5 Water  
CON overnight, room temperature

RX(14) OF 57 ...M + AE ==> AI



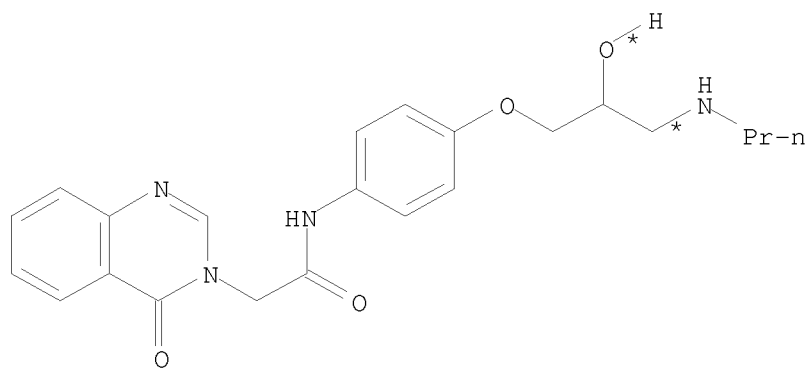
M



AE

(14)  
→

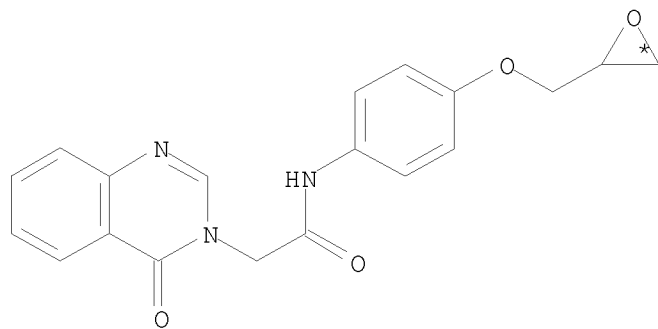
10/ 562,112



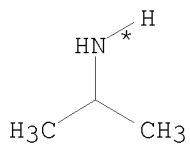
AI  
YIELD 36%

RX(14) RCT M 107-10-8, AE 864234-49-1  
PRO AI 864234-51-5  
CON 6 hours, reflux  
NTE no solvent

RX(15) OF 57 ...AE + AJ ==> AK



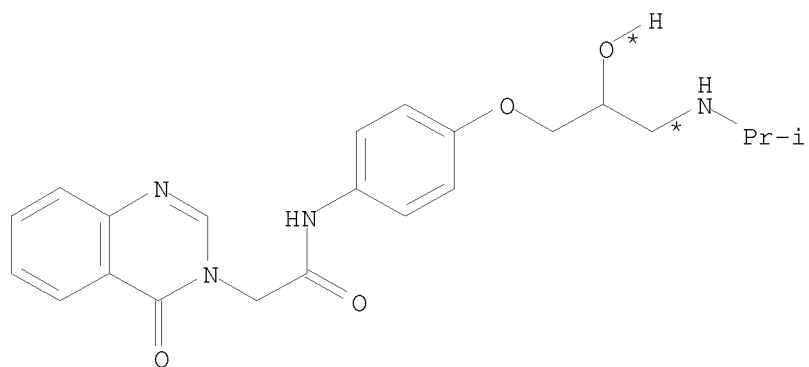
AE



AJ

(15)  $\longrightarrow$

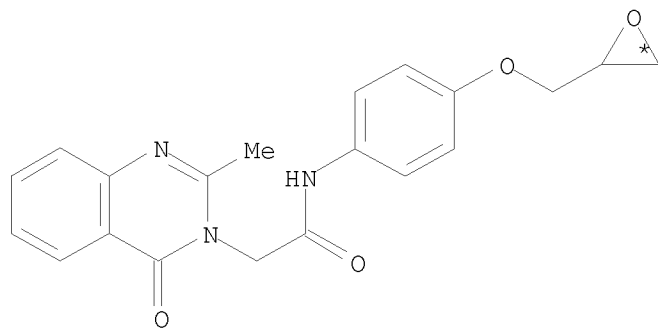
10/ 562,112



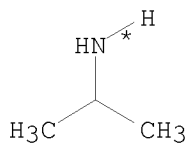
AK  
YIELD 30%

RX(15)      RCT    AE 864234-49-1, AJ 75-31-0  
              PRO    AK 864234-52-6  
              SOL    68-12-2 DMF  
              CON    6 hours, reflux

RX(16) OF 57      ...AH    +    AJ    ==>    AM



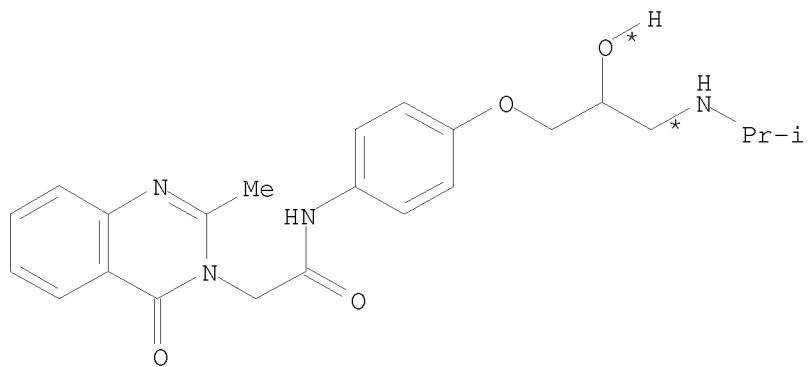
AH



AJ

(16)  $\longrightarrow$

10/ 562,112

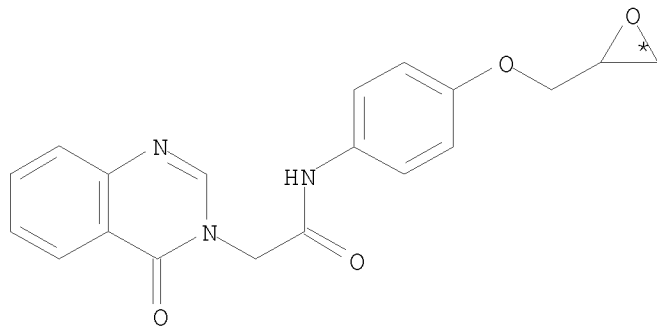


AM

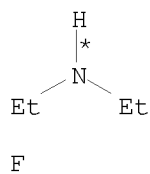
YIELD 32%

RX(16) RCT AH 864234-50-4, AJ 75-31-0  
PRO AM 864234-53-7  
SOL 68-12-2 DMF  
CON 6 hours, reflux

RX(17) OF 57 ...AE + F ==> AN

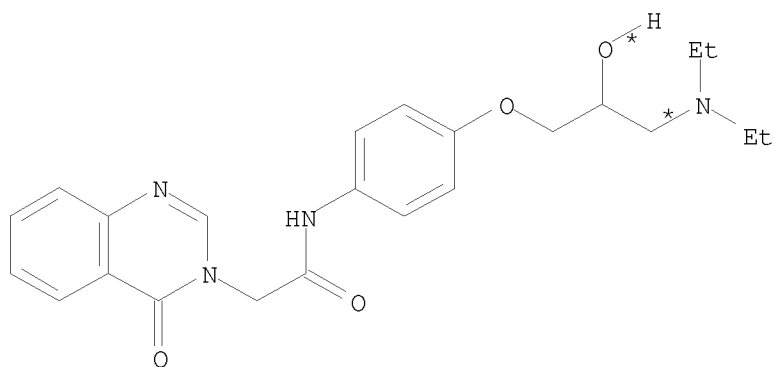


AE



(17)  $\longrightarrow$

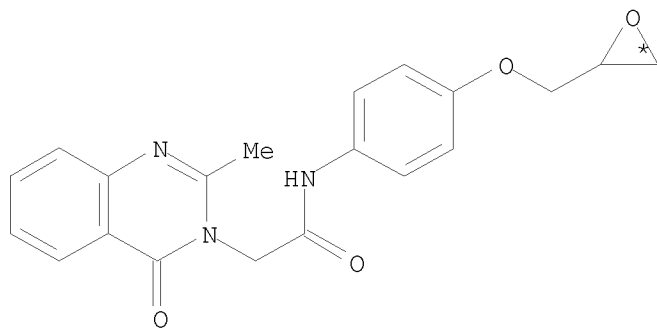
10/ 562,112



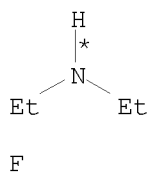
AN  
YIELD 28%

RX(17)      RCT    AE 864234-49-1, F 109-89-7  
              PRO    AN 864234-54-8  
              SOL    68-12-2 DMF  
              CON    6 hours, reflux

RX(18) OF 57      ...AH    +    F    ==>    AO



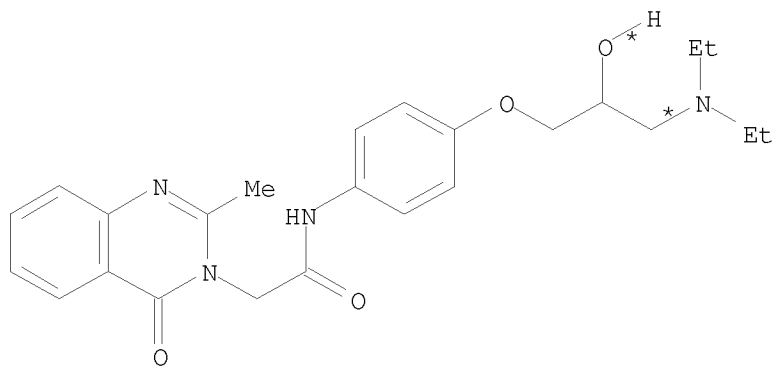
AH



(18)  $\longrightarrow$



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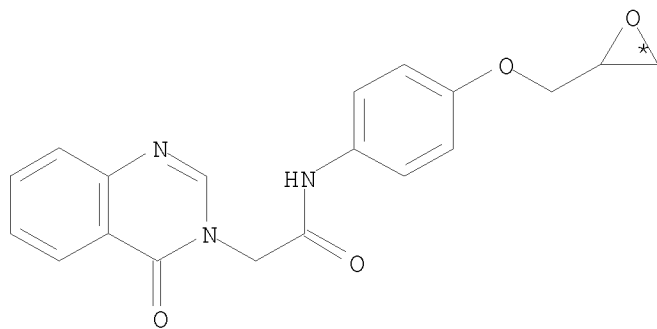


AO

YIELD 35%

RX(18)      RCT    AH 864234-50-4, F 109-89-7  
              PRO    AO 864234-55-9  
              SOL    68-12-2 DMF  
              CON    6 hours, reflux

RX(19) OF 57      ...AE + AP ==> AQ

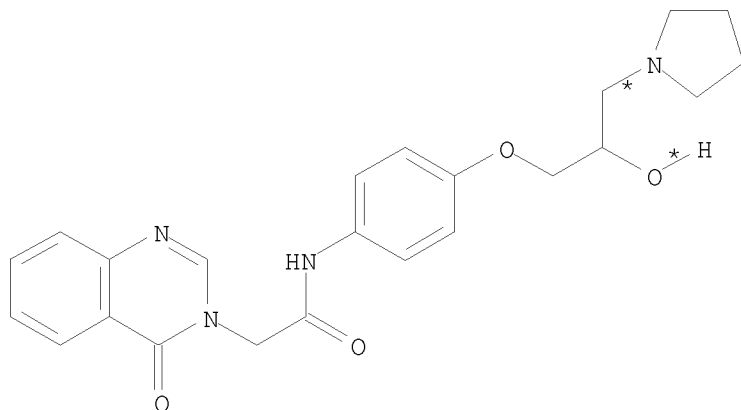


AE

AP

(19)  $\longrightarrow$

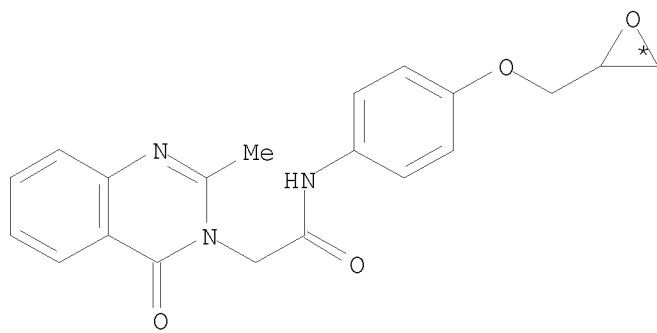
10/ 562,112



AQ  
YIELD 36%

RX(19)      RCT    AE 864234-49-1, AP 123-75-1  
              PRO    AQ 864234-56-0  
              CON    6 hours, reflux  
              NTE    no solvent

RX(20) OF 57      ...AH    +    AP    ==>    AR

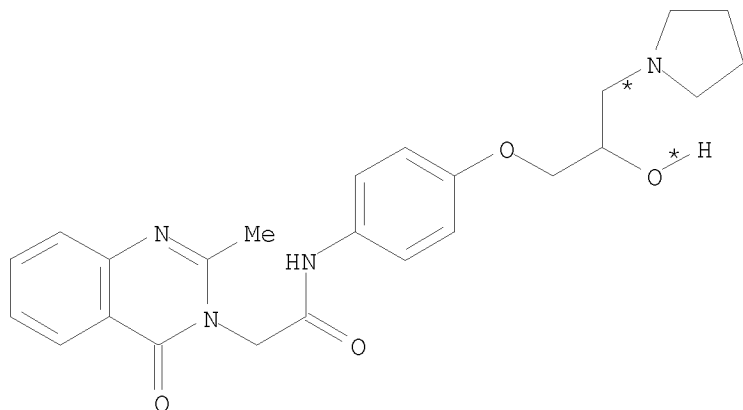


AH

AP

(20)  $\longrightarrow$

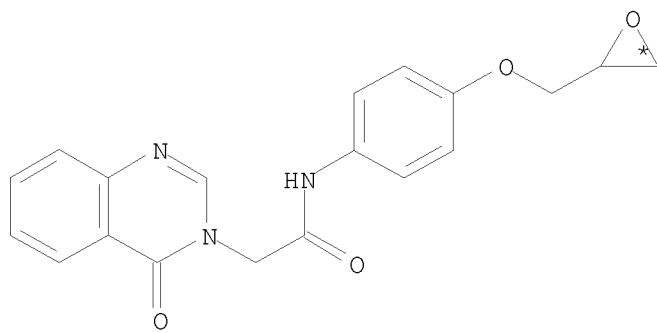
10/ 562,112



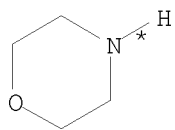
AR  
YIELD 42%

RX(20)      RCT    AH 864234-50-4, AP 123-75-1  
              PRO    AR 864234-57-1  
              CON    6 hours, reflux  
              NTE    no solvent

RX(21) OF 57      ...AE + AS ==> AT



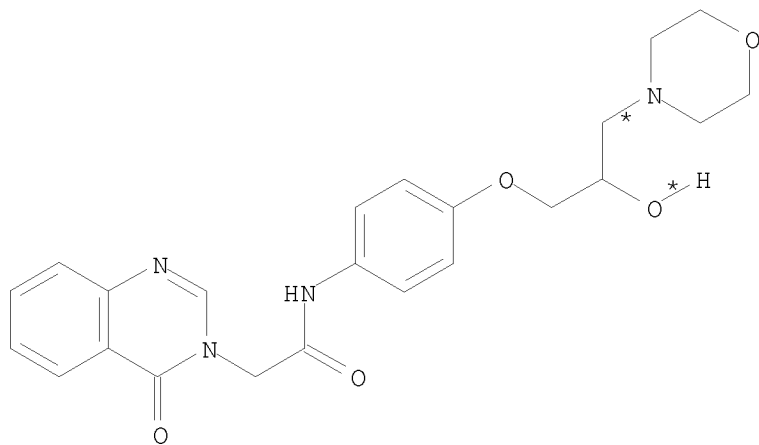
AE



AS

(21)  $\longrightarrow$

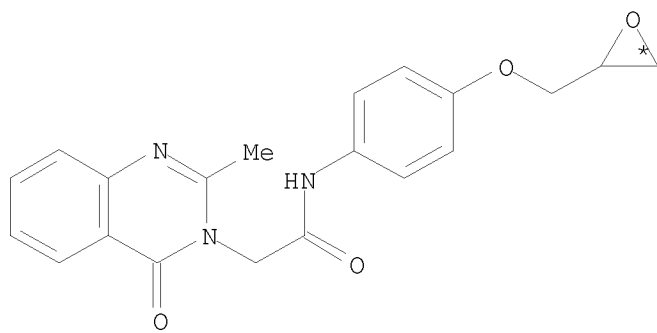
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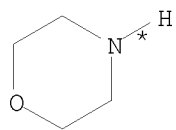
AT  
YIELD 30%

RX(21)     RCT   AE 864234-49-1, AS 110-91-8  
             PRO   AT 864234-58-2  
             CON   6 hours, reflux  
             NTE   no solvent

RX(22) OF 57     ...AH   +   AS   ==>   AU



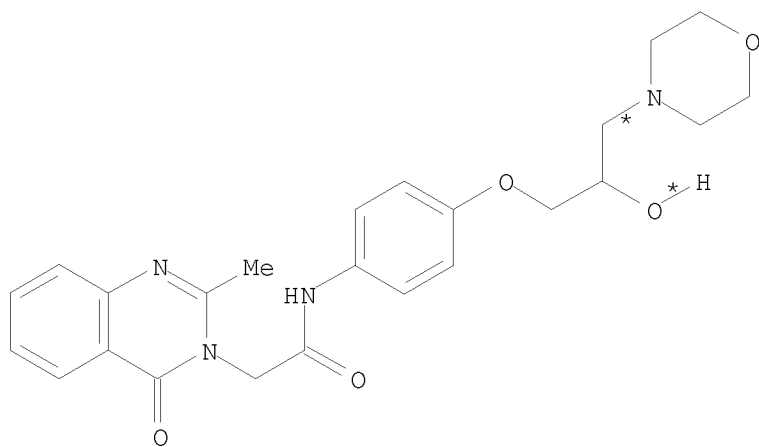
AH



AS

(22)  
→

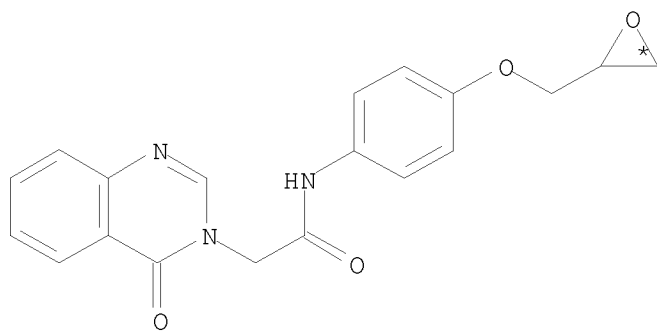
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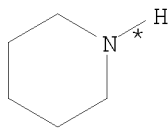
AU  
YIELD 20%

RX(22)     RCT    AH 864234-50-4, AS 110-91-8  
             PRO    AU 864234-59-3  
             CON    6 hours, reflux  
             NTE    no solvent

RX(23) OF 57     ...AE   +   AV   ==>   AW



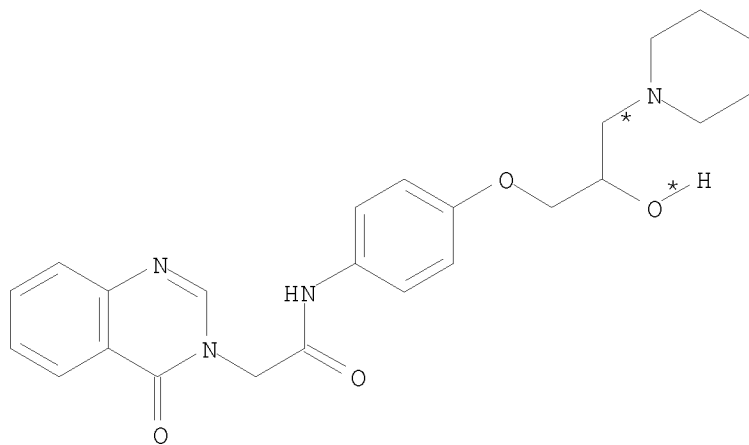
AE



AV

(23)  $\longrightarrow$

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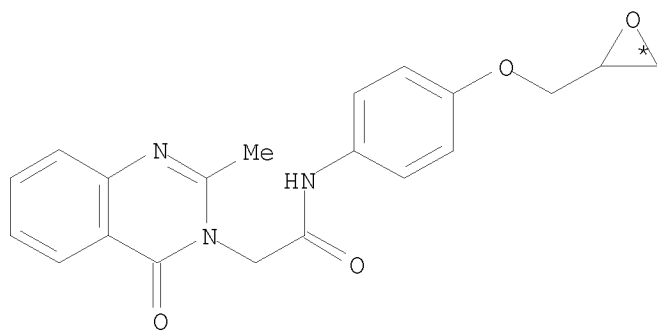


AW

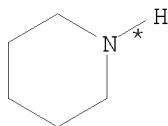
YIELD 45%

RX(23)     RCT   AE 864234-49-1, AV 110-89-4  
             PRO   AW 864234-60-6  
             CON   6 hours, reflux  
             NTE   no solvent

RX(24) OF 57     ...AH   +   AV   ==>   AX



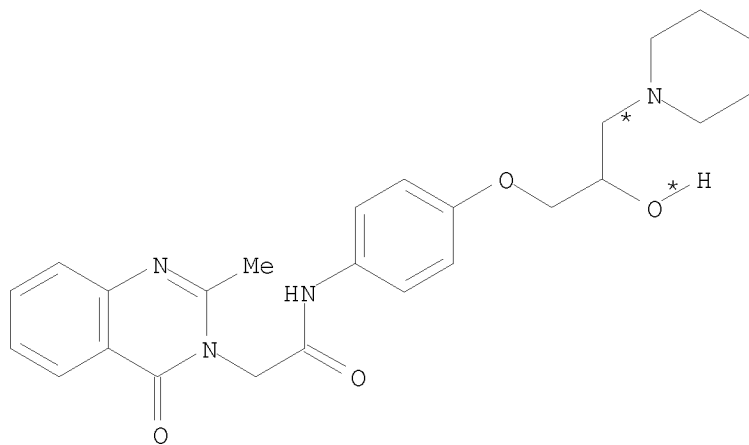
AH



AV

(24)

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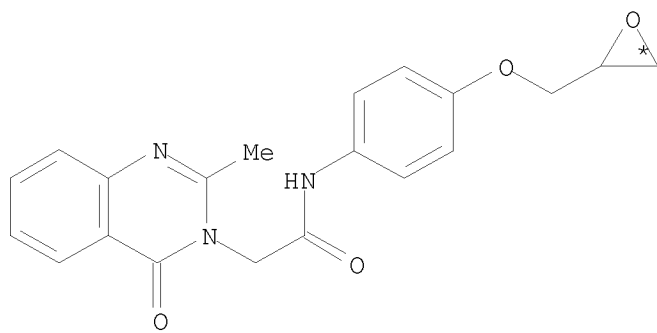


AX

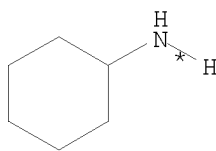
YIELD 35%

RX(24)     RCT    AH 864234-50-4, AV 110-89-4  
             PRO    AX 864234-61-7  
             CON    6 hours, reflux  
             NTE    no solvent

RX(25) OF 57     ...AH   +   AY   ==>   AZ



AH

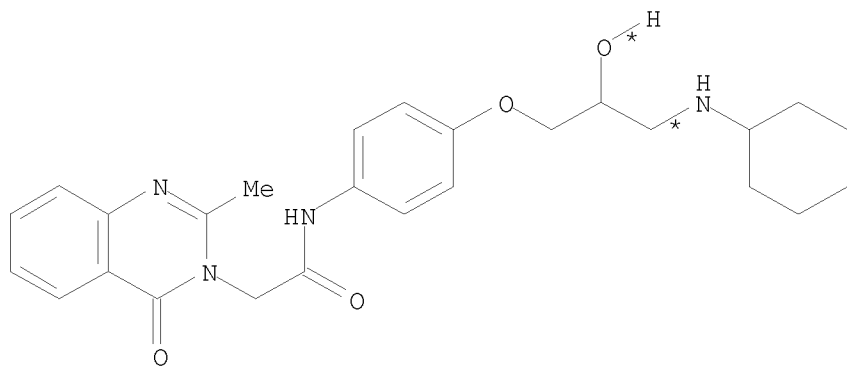


AY

(25)



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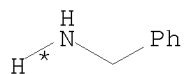


AZ

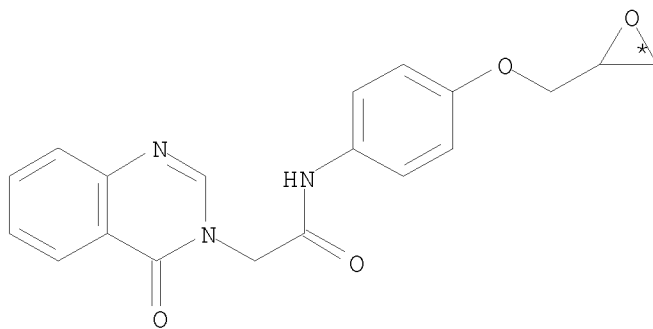
YIELD 32%

RX(25)      RCT    AH 864234-50-4, AY 108-91-8  
              PRO    AZ 864234-62-8  
              CON    6 hours, reflux  
              NTE    no solvent

RX(26) OF 57      ...B + AE ==> BA



B

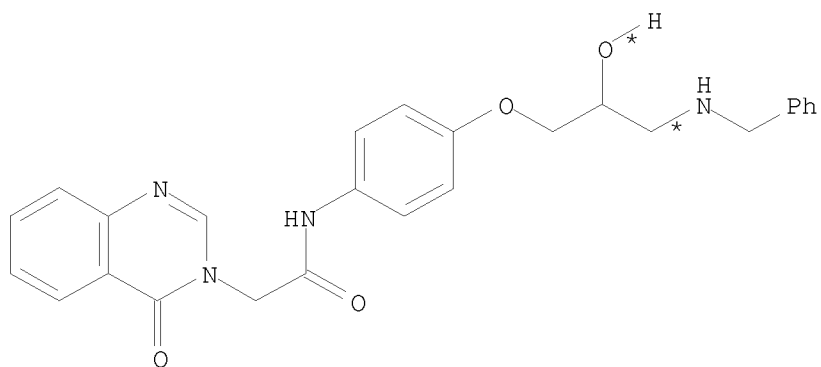


AE

(26)



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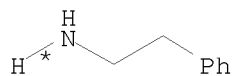


BA

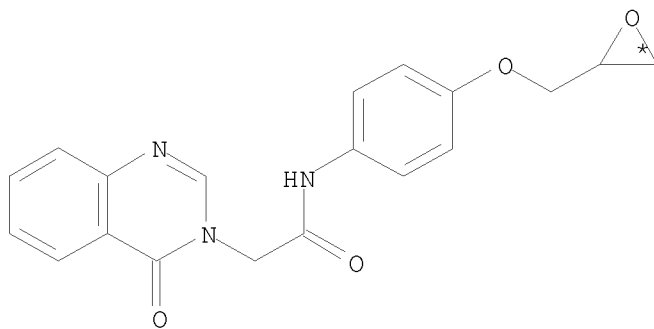
YIELD 40%

RX(26)      RCT    B 100-46-9, AE 864234-49-1  
              PRO    BA 864234-63-9  
              CON    6 hours, reflux  
              NTE    no solvent

RX(27) OF 57      ...K + AE ==> BB



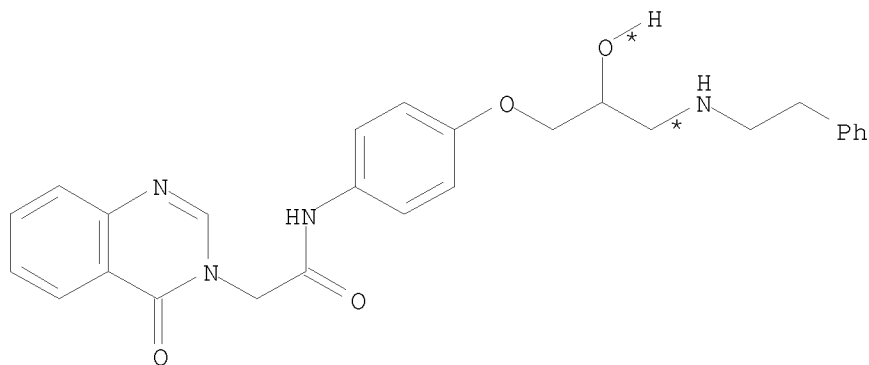
K



AE

(27)  $\longrightarrow$

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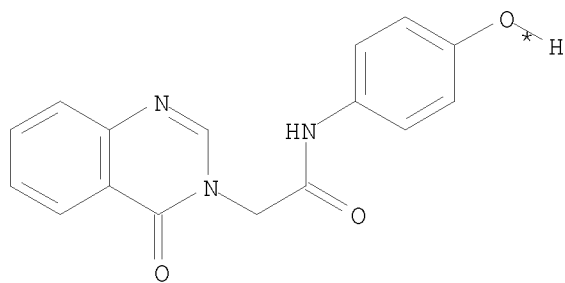


BB

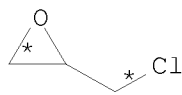
YIELD 25%

RX(27)      RCT    K 64-04-0, AE 864234-49-1  
             PRO    BB 864234-64-0  
             CON    6 hours, reflux  
             NTE    no solvent

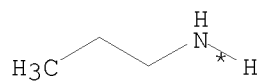
RX(30) OF 57 COMPOSED OF RX(12), RX(14)  
RX(30)      Z    +    AD    +    M    ==>    AI



Z



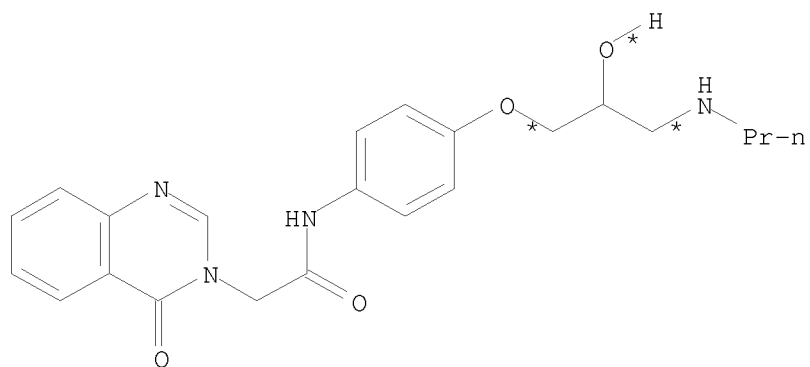
AD



M

2  
STEPS  
=>

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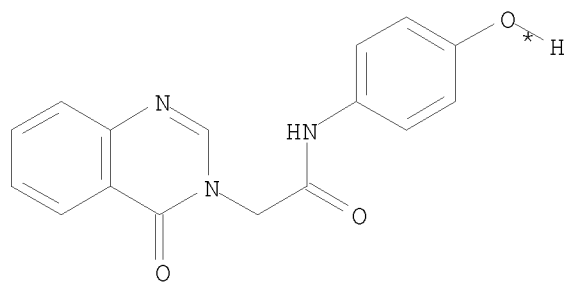


AI  
YIELD 36%

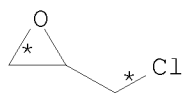
RX(12)      RCT    Z 591213-29-5, AD 106-89-8  
              RGT    AF 1310-58-3 KOH  
              PRO    AE 864234-49-1  
              SOL    7732-18-5 Water  
              CON    overnight, room temperature

RX(14)      RCT    M 107-10-8, AE 864234-49-1  
              PRO    AI 864234-51-5  
              CON    6 hours, reflux  
              NTE    no solvent

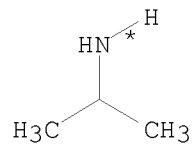
RX(31) OF 57 COMPOSED OF RX(12), RX(15)  
RX(31)      Z    +    AD    +    AJ    ==>    AK



Z

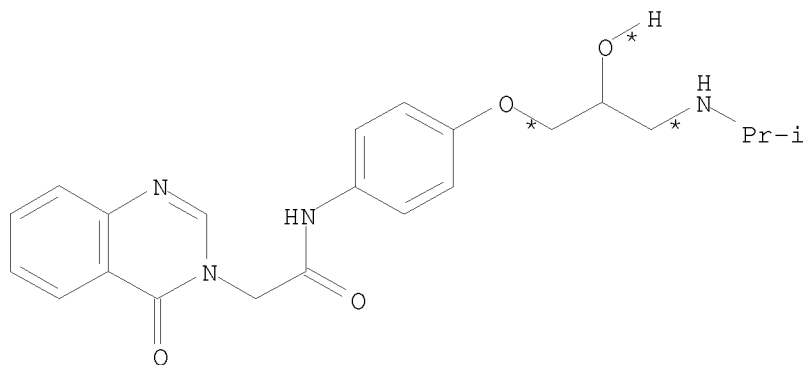


AD



AJ

2  
STEPS  
→

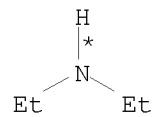
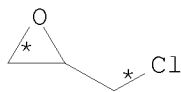
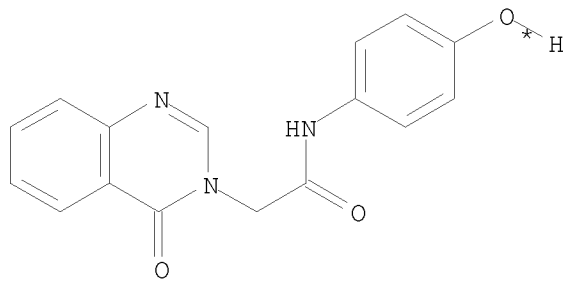


AK  
YIELD 30%

RX(12) RCT Z 591213-29-5, AD 106-89-8  
RGT AF 1310-58-3 KOH  
PRO AE 864234-49-1  
SOL 7732-18-5 Water  
CON overnight, room temperature

RX(15)      RCT    AE 864234-49-1, AJ 75-31-0  
              PRO    AK 864234-52-6  
              SOL    68-12-2 DMF  
              CON    6 hours, reflux

RX(32) OF 57 COMPOSED OF RX(12), RX(17)  
 RX(32) Z + AD + F ==> AN

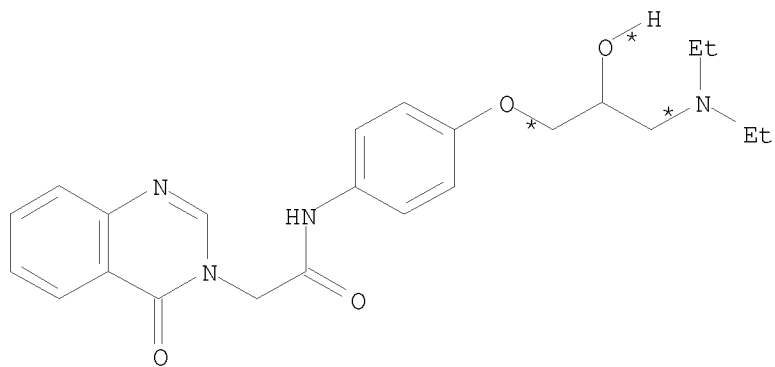


Z

AD

F

2  
STEPS  
→

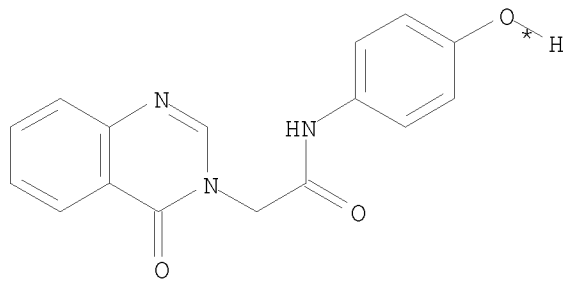


AN  
YIELD 28%

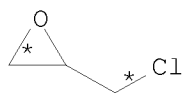
RX(12) RCT Z 591213-29-5, AD 106-89-8  
RGT AF 1310-58-3 KOH  
PRO AE 864234-49-1  
SOL 7732-18-5 Water  
CON overnight, room temperature

RX(17)      RCT    AE 864234-49-1, F 109-89-7  
               PRO    AN 864234-54-8  
               SOL    68-12-2 DMF  
               CON    6 hours, reflux

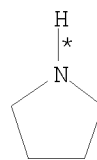
RX(33) OF 57 COMPOSED OF RX(12), RX(19)  
 RX(33) Z + AD + AP ==> AQ



Z



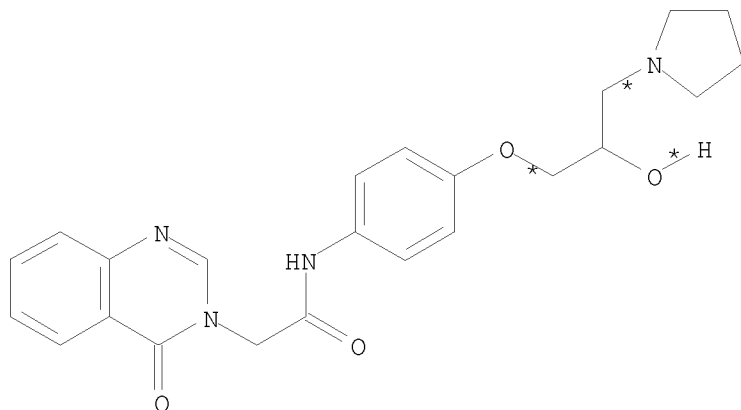
AD



AP

2  
STEPS  
→

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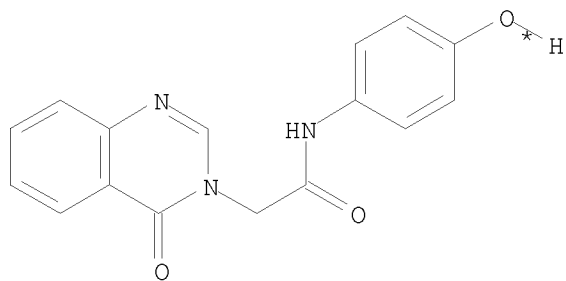


AQ  
YIELD 36%

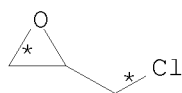
RX(12)     RCT    Z 591213-29-5, AD 106-89-8  
             RGT    AF 1310-58-3 KOH  
             PRO    AE 864234-49-1  
             SOL    7732-18-5 Water  
             CON    overnight, room temperature

RX(19)     RCT    AE 864234-49-1, AP 123-75-1  
             PRO    AQ 864234-56-0  
             CON    6 hours, reflux  
             NTE    no solvent

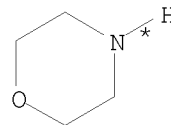
RX(34) OF 57 COMPOSED OF RX(12), RX(21)  
RX(34)     Z    +    AD    +    AS    ==>    AT



Z



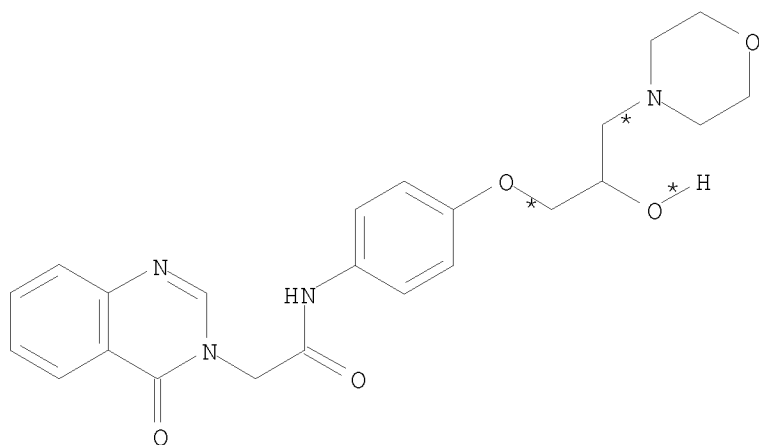
AD



AS

2  
STEPS  
=>

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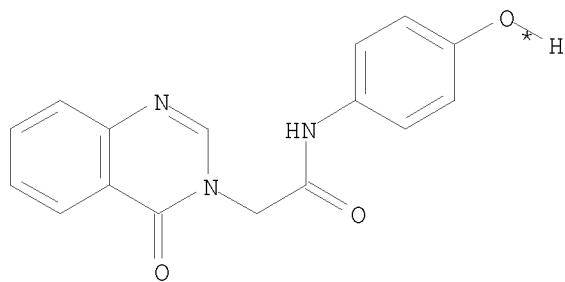


AT  
YIELD 30%

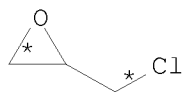
RX(12) RCT Z 591213-29-5, AD 106-89-8  
RGT AF 1310-58-3 KOH  
PRO AE 864234-49-1  
SOL 7732-18-5 Water  
CON overnight, room temperature

RX(21) RCT AE 864234-49-1, AS 110-91-8  
PRO AT 864234-58-2  
CON 6 hours, reflux  
NTE no solvent

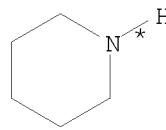
RX(35) OF 57 COMPOSED OF RX(12), RX(23)  
RX(35) Z + AD + AV ==> AW



Z



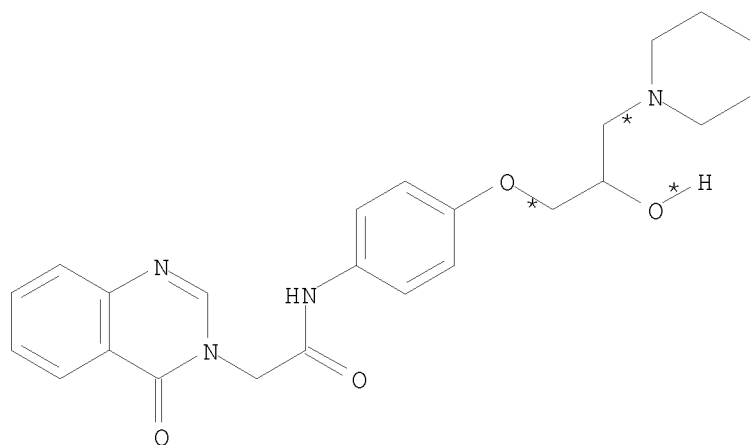
AD



AV

2  
STEPS  
→

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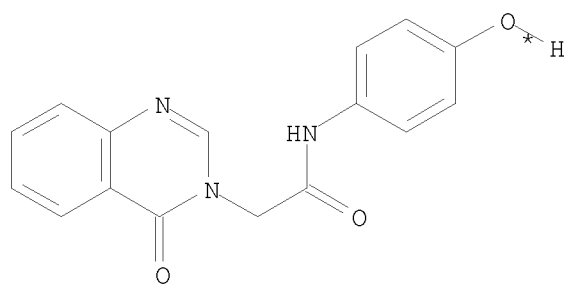


AW  
YIELD 45%

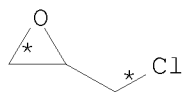
RX(12) RCT Z 591213-29-5, AD 106-89-8  
RGT AF 1310-58-3 KOH  
PRO AE 864234-49-1  
SOL 7732-18-5 Water  
CON overnight, room temperature

RX(23) RCT AE 864234-49-1, AV 110-89-4  
PRO AW 864234-60-6  
CON 6 hours, reflux  
NTE no solvent

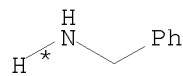
RX(36) OF 57 COMPOSED OF RX(12), RX(26)  
RX(36) Z + AD + B ==> BA



Z



AD

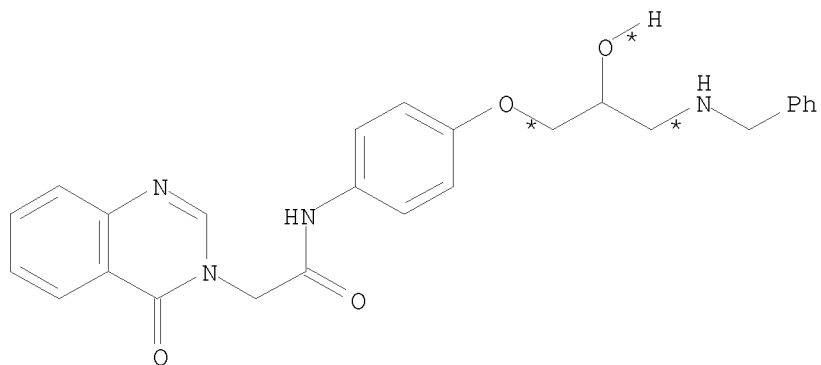


B

2  
STEPS  
→



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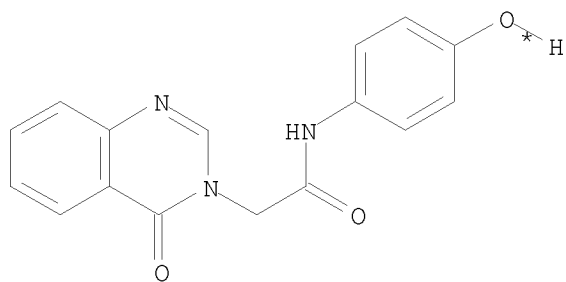


BA  
YIELD 40%

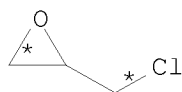
RX(12) RCT Z 591213-29-5, AD 106-89-8  
RGT AF 1310-58-3 KOH  
PRO AE 864234-49-1  
SOL 7732-18-5 Water  
CON overnight, room temperature

RX(26) RCT B 100-46-9, AE 864234-49-1  
PRO BA 864234-63-9  
CON 6 hours, reflux  
NTE no solvent

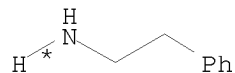
RX(37) OF 57 COMPOSED OF RX(12), RX(27)  
RX(37) Z + AD + K ==> BB



Z

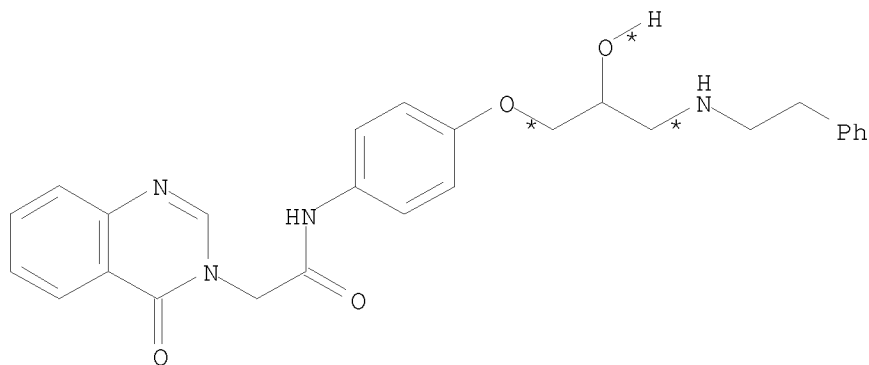


AD



K

2  
STEPS  
→



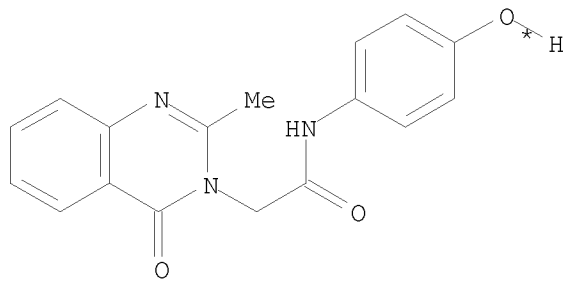
BB

YIELD 25%

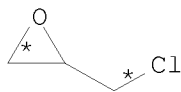
RX(12) RCT Z 591213-29-5, AD 106-89-8  
RGT AF 1310-58-3 KOH  
PRO AE 864234-49-1  
SOL 7732-18-5 Water  
CON overnight, room temperature

RX(27)	RCT	K 64-04-0, AE 864234-49-1
	PRO	BB 864234-64-0
	CON	6 hours, reflux
	NTE	no solvent

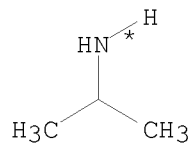
RX(38) OF 57 COMPOSED OF RX(13), RX(16)  
RX(38) AC + AD + AJ ==> AM



AC



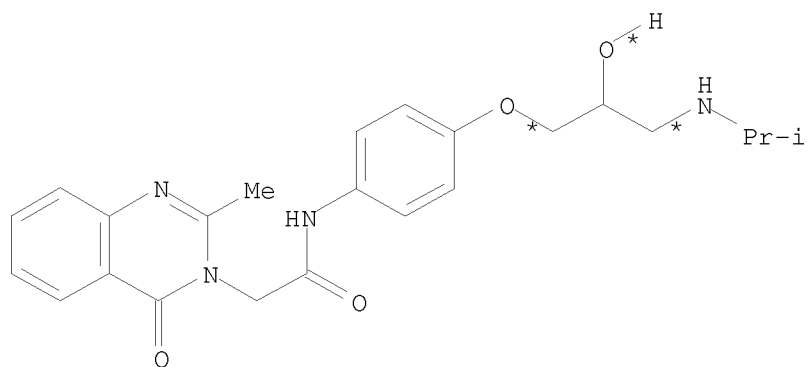
AD



AJ

2  
STEPS  
→

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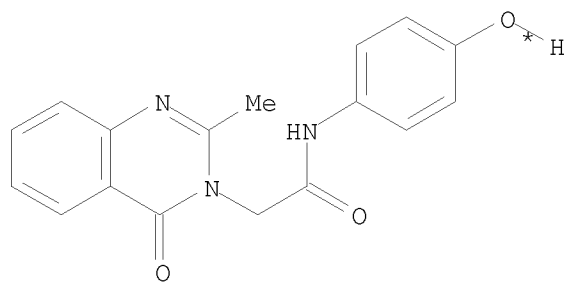


AM  
YIELD 32%

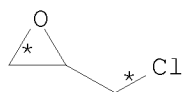
RX(13)      RCT    AC 864234-48-0, AD 106-89-8  
              RGT    AF 1310-58-3 KOH  
              PRO    AH 864234-50-4  
              SOL    7732-18-5 Water  
              CON    overnight, room temperature

RX(16)      RCT    AH 864234-50-4, AJ 75-31-0  
              PRO    AM 864234-53-7  
              SOL    68-12-2 DMF  
              CON    6 hours, reflux

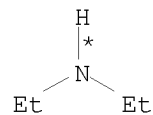
RX(39) OF 57 COMPOSED OF RX(13), RX(18)  
RX(39)      AC + AD + F ==> AO



AC



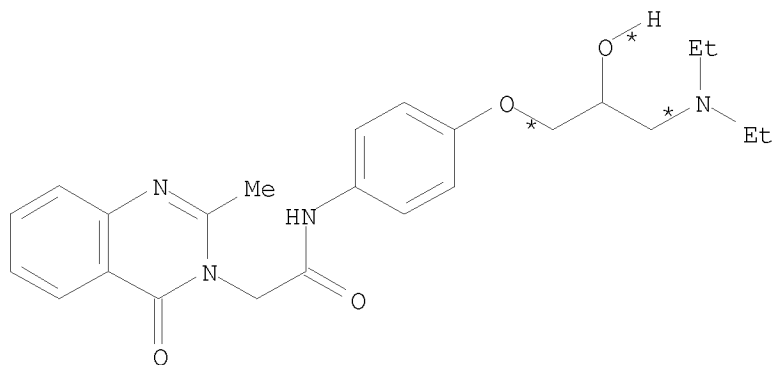
AD



F

2  
STEPS  
→

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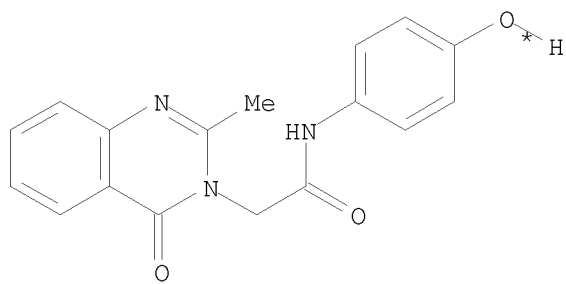


AO  
YIELD 35%

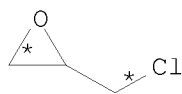
RX(13) RCT AC 864234-48-0, AD 106-89-8  
RGT AF 1310-58-3 KOH  
PRO AH 864234-50-4  
SOL 7732-18-5 Water  
CON overnight, room temperature

RX(18) RCT AH 864234-50-4, F 109-89-7  
PRO AO 864234-55-9  
SOL 68-12-2 DMF  
CON 6 hours, reflux

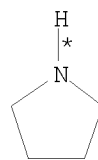
RX(40) OF 57 COMPOSED OF RX(13), RX(20)  
RX(40) AC + AD + AP ==> AR



AC



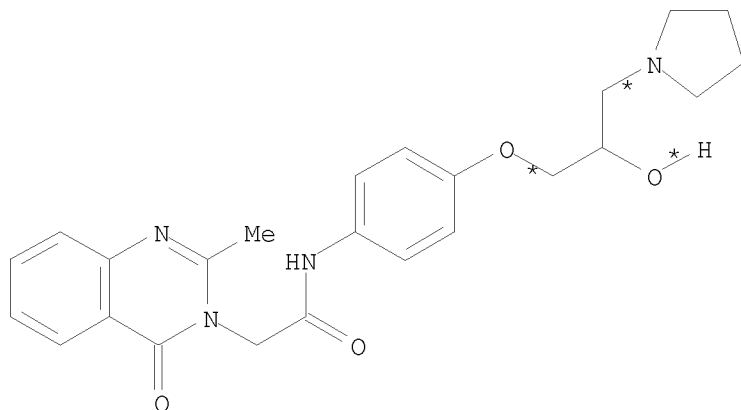
AD



AP

2  
STEPS  
→

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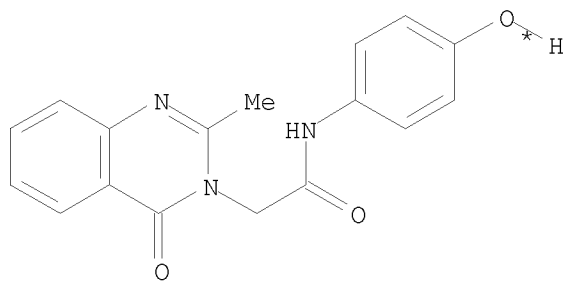


AR  
YIELD 42%

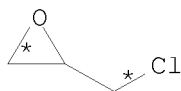
RX(13) RCT AC 864234-48-0, AD 106-89-8  
RGT AF 1310-58-3 KOH  
PRO AH 864234-50-4  
SOL 7732-18-5 Water  
CON overnight, room temperature

RX(20) RCT AH 864234-50-4, AP 123-75-1  
PRO AR 864234-57-1  
CON 6 hours, reflux  
NTE no solvent

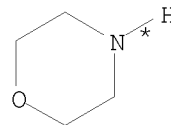
RX(41) OF 57 COMPOSED OF RX(13), RX(22)  
RX(41) AC + AD + AS ==> AU



AC



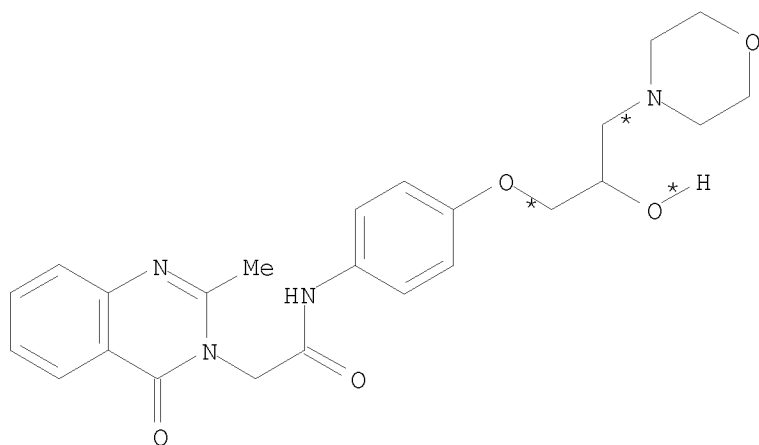
AD



AS

2  
STEPS  
=>

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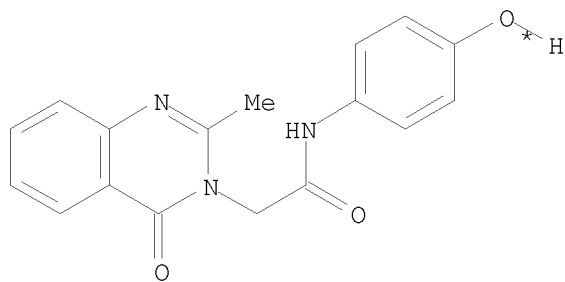
AU  
YIELD 20%

RX(13) RCT AC 864234-48-0, AD 106-89-8  
RGT AF 1310-58-3 KOH  
PRO AH 864234-50-4  
SOL 7732-18-5 Water  
CON overnight, room temperature

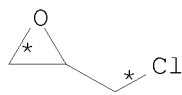
RX(22) RCT AH 864234-50-4, AS 110-91-8  
PRO AU 864234-59-3  
CON 6 hours, reflux  
NTE no solvent

RX(42) OF 57 COMPOSED OF RX(13), RX(24)

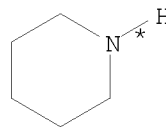
RX(42) AC + AD + AV ==> AX



AC



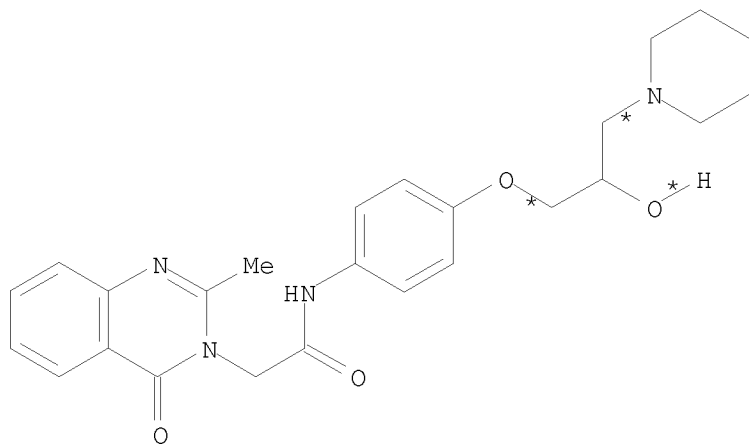
AD



AV

2  
STEPS  
→

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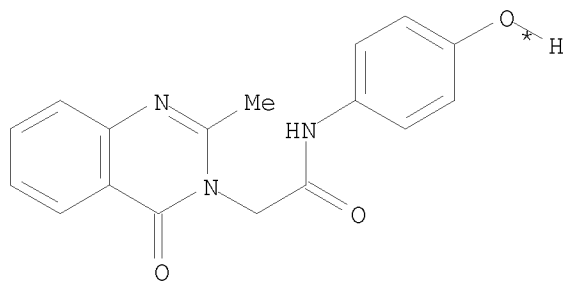


AX  
YIELD 35%

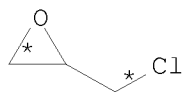
RX(13) RCT AC 864234-48-0, AD 106-89-8  
RGT AF 1310-58-3 KOH  
PRO AH 864234-50-4  
SOL 7732-18-5 Water  
CON overnight, room temperature

RX(24) RCT AH 864234-50-4, AV 110-89-4  
PRO AX 864234-61-7  
CON 6 hours, reflux  
NTE no solvent

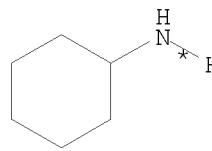
RX(43) OF 57 COMPOSED OF RX(13), RX(25)  
RX(43) AC + AD + AY ==> AZ



AC

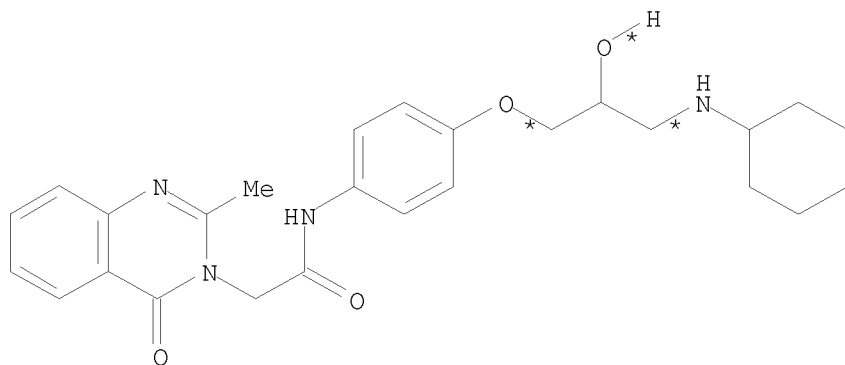


AD



AY

2  
STEPS  
→



AZ  
YIELD 32%

RX(13) RCT AC 864234-48-0, AD 106-89-8  
RGT AF 1310-58-3 KOH  
PRO AH 864234-50-4  
SOL 7732-18-5 Water  
CON overnight, room temperature

RX(25) RCT AH 864234-50-4, AY 108-91-8  
PRO AZ 864234-62-8  
CON 6 hours, reflux  
NTE no solvent

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 47 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 143:211923 CASREACT  
TITLE: Preparation of fused-ring 4-oxopyrimidine derivatives  
as histamine H3 receptor antagonists or inverse  
agonists  
INVENTOR(S): Nagase, Tsuyoshi; Sato, Nagaaki; Kanatani, Akio;  
Tokita, Shigeru  
PATENT ASSIGNEE(S): Banyu Pharmaceutical Co., Ltd., Japan  
SOURCE: U.S. Pat. Appl. Publ., 84 pp.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050182045	A1	20050818	US 2005-58444	20050214
AU 2005212092	A1	20050825	AU 2005-212092	20050214
CA 2555824	A1	20050825	CA 2005-2555824	20050214
WO 2005077905	A1	20050825	WO 2005-JP2664	20050214

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,



GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

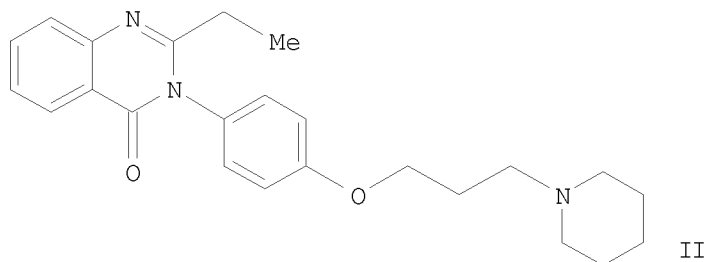
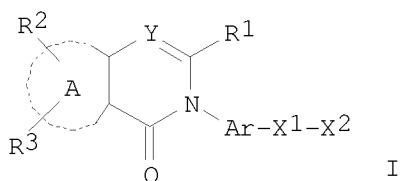
EP 1717230 A1 20061102 EP 2005-710446 20050214  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR, IS

CN 1918128 A 20070221 CN 2005-80004939 20050214  
 BR 2005007629 A 20070703 BR 2005-7629 20050214  
 JP 4102939 B2 20080618 JP 2005-518071 20050214  
 MX 2006009244 A 20061110 MX 2006-9244 20060811  
 NO 2006004089 A 20061106 NO 2006-4089 20060912  
 IN 2006DN05284 A 20070803 IN 2006-DN5284 20060913  
 JP 2008156358 A 20080710 JP 2007-335972 20071227

PRIORITY APPLN. INFO.:

JP 2004-37190 20040213  
 JP 2005-518071 20050214  
 WO 2005-JP2664 20050214

OTHER SOURCE(S): MARPAT 143:211923  
 GI

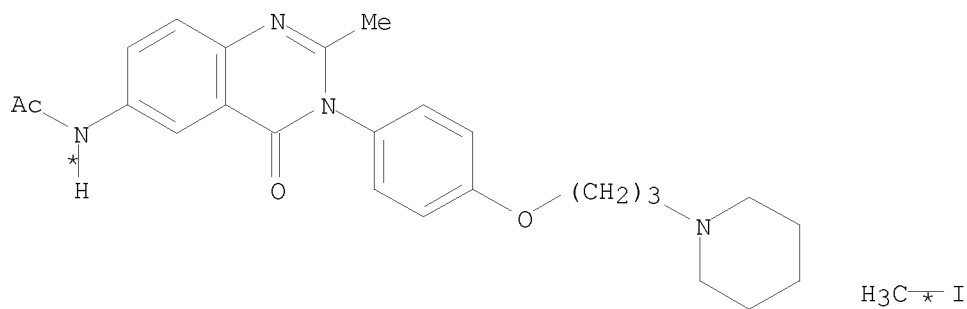


AB The present invention provides fused-ring 4-oxopyrimidines (shown as I; variables defined below; e.g. 2-ethyl-3-[4-[3-(1-piperidinyl)propoxy]phenyl]-4(3H)-quinazolinone (shown as II)) or pharmaceutically acceptable salts thereof, which, having histamine H3 receptor antagonist or inverse agonist activity, are useful in the prophylaxis or therapy of metabolic diseases, circulatory diseases, or nervous system diseases. For I: e.g. Ar is a divalent group formed by eliminating two H atoms from benzene; X1 = N, S, or O; R1 is a 5- to 6-membered heteroaryl group; Ring A is a 5- to 6-membered heteroaryl ring; R2 and R3 are amino or alkylamino groups; Y = CH or N; and X2 = -(CH2)<sub>n</sub>NR4R5 (R4 and R5 are lower alkyl groups, and n = 2-4). Although the methods of preparation are not claimed, .aprx.275 example preps. are

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included. For example, II was prepared in 4 steps (98, 66, 82 and 47 %) starting from anthranilic acid and propionic anhydride and involving intermediates 2-ethyl-4H-3,1-benzoxazin-4-one, 2-ethyl-3-(4-hydroxyphenyl)-4(3H)-quinazolinone, and 2-ethyl-3-[4-(3-chloropropoxy)phenyl]-4(3H)-quinazolinone. Pharmacol. results are provided for II for the following tests: histamine analog coupling inhibition, antagonism of drinking behavior induced by R- $\alpha$ -methylhistamine (a histamine H3 receptor selective agonist), in vitro kinetics, and brain/cerebrospinal fluid activity.

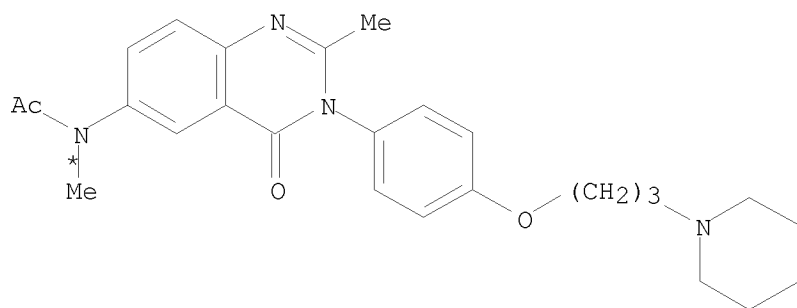
RX(97) OF 861 ...EW + FV ==> FW



EW

FV

(97)  
→



FW

RX(97) RCT EW 862309-53-3

STAGE(1)

RGT BM 7646-69-7 NaH

STAGE(2)

RCT FV 74-88-4

SOL 109-99-9 THF, 110-86-1 Pyridine

CON SUBSTAGE(1) cooled

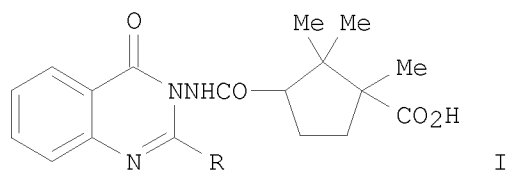
SUBSTAGE(2) cooled

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SUBSTAGE(3) overnight, room temperature

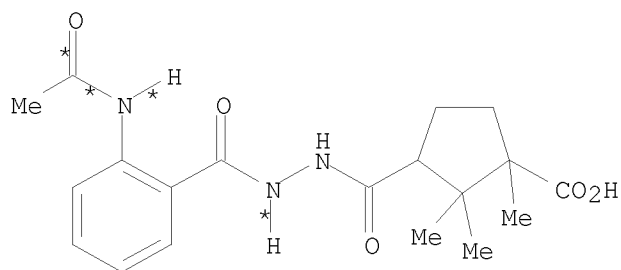
PRO FW 862309-89-5

L3 ANSWER 48 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 143:172829 CASREACT  
TITLE: Synthesis of ( $\pm$ )-1,2,2-trimethyl-1,3-cyclopentanedicarboxylic acid derivatives with a 4(3H)-quinazolinone fragment  
AUTHOR(S): Gritsenko, I. S.; Tsapko, Ye. A.  
CORPORATE SOURCE: Nats. Farm. Univ., Kharkov, 61146, Ukraine  
SOURCE: Zhurnal Organichnoi ta Farmatsevtichnoi Khimii (2005), 3(1), 12-16  
CODEN: ZOFKAM  
PUBLISHER: Natsional'nii Farmatsevtichnii Universitet  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
GI



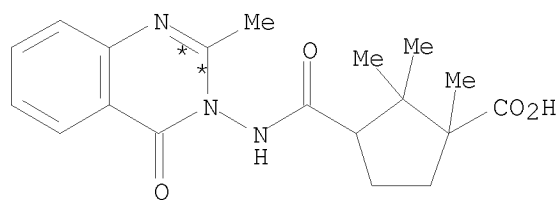
AB The hydrazide of anthranilic acid has been acylated by 1,2,2-trimethylcyclopentanedicarboxylic acid anhydride. The product of the reaction was cyclized to the title compds. (I; R = Me, Et, Pr, CC13).

RX(14) OF 64 ...G ==> N...



(14)

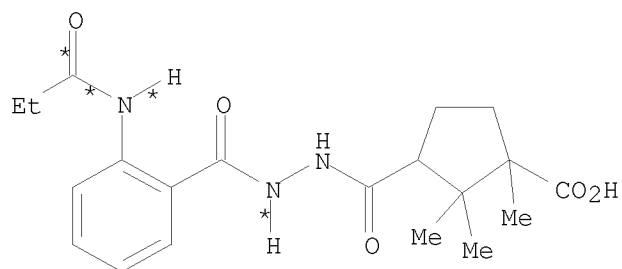
10/ 562,112



N  
YIELD 83%

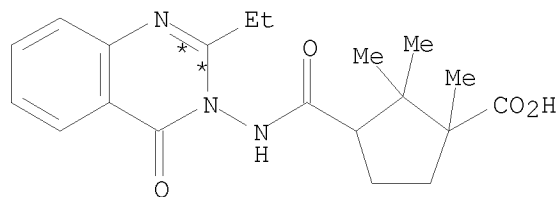
RX(14)     RCT   G 860479-66-9  
           RGT   V 68-12-2 DMF  
           PRO   N 860479-70-5  
           SOL   1330-20-7 Xylene  
           CON   15 - 20 minutes, reflux  
           NTE   regioselective, alternative preparation shown, brombenzene/agent  
                 gave similar results

RX(15) OF 64     ...I   ==>   P...



I

(15)  
→



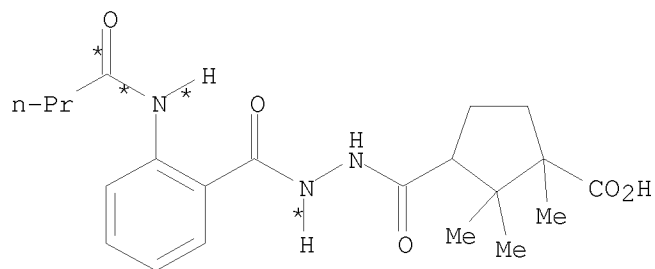
P  
YIELD 78%

RX(15)     RCT   I 860479-67-0  
           RGT   V 68-12-2 DMF  
           PRO   P 860479-71-6  
           SOL   1330-20-7 Xylene  
           CON   15 - 20 minutes, reflux  
           NTE   regioselective, alternative preparation shown, brombenzene/agent

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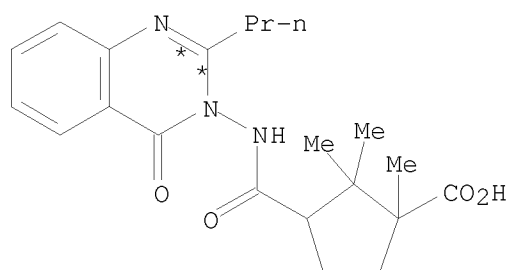
gave similar results

RX(16) OF 64      ...K ==> Q...



K

(16)  
→



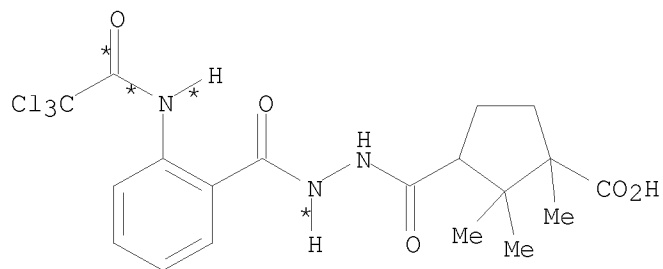
Q

YIELD 69%

RX(16)      RCT    K 860479-68-1  
             RGT    V 68-12-2 DMF  
             PRO    Q 860479-72-7  
             SOL    1330-20-7 Xylene  
             CON    SUBSTAGE(1) 15 - 20 minutes, reflux  
                     SUBSTAGE(2) cooled  
             NTE    regioselective, alternative preparation shown, brombenzene/agent  
                     gave similar results

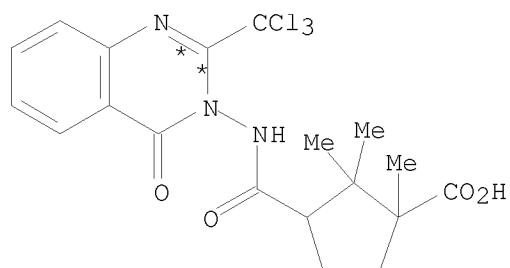
RX(17) OF 64      ...M ==> R

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M

(17)  $\longrightarrow$

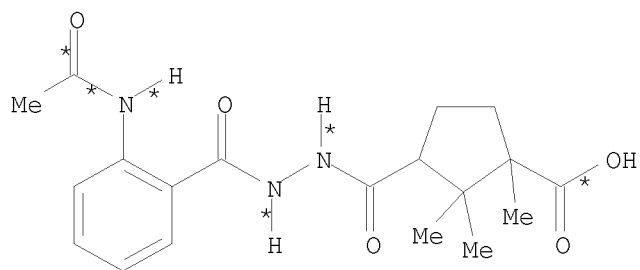


R

YIELD 76%

RX(17)     RCT   M 860479-69-2  
              RGT   V 68-12-2 DMF  
              PRO   R 860479-73-8  
              SOL   1330-20-7 Xylene  
              CON   15 - 20 minutes, reflux  
              NTE   regioselective, alternative preparation shown, brombenzene/agent  
                      gave similar results

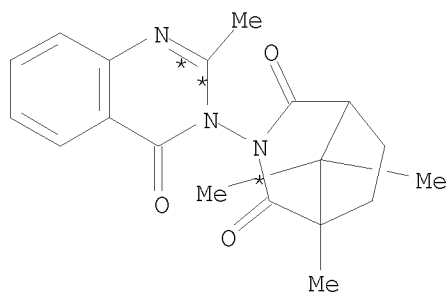
RX(19) OF 64     ...G    $\implies$    S



G

(19)  $\longrightarrow$

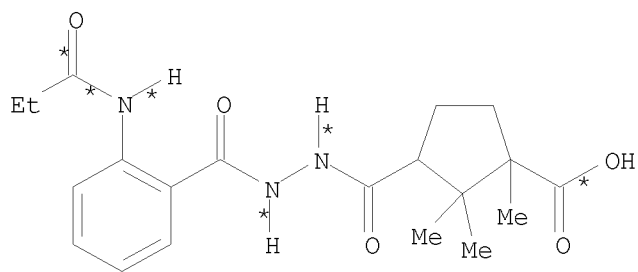
10/ 562,112



S  
YIELD 88%

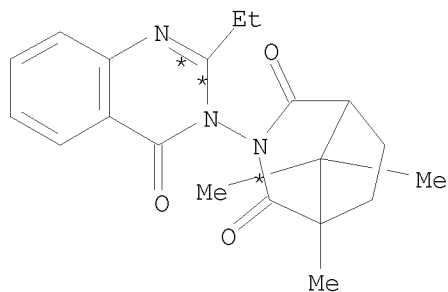
RX(19)      RCT    G 860479-66-9  
             PRO    S 860479-74-9  
             CON    45 minutes, 220 - 230 deg C  
             NTE    regioselective, thermal, alternative preparation shown, no solvent

RX(21) OF 64      ...I    ==>    T



I

(21)  
→



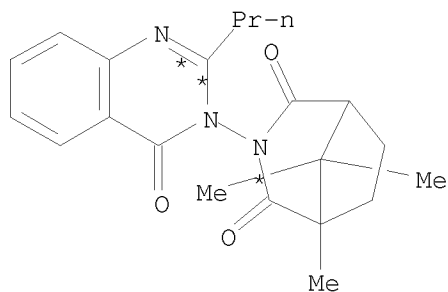
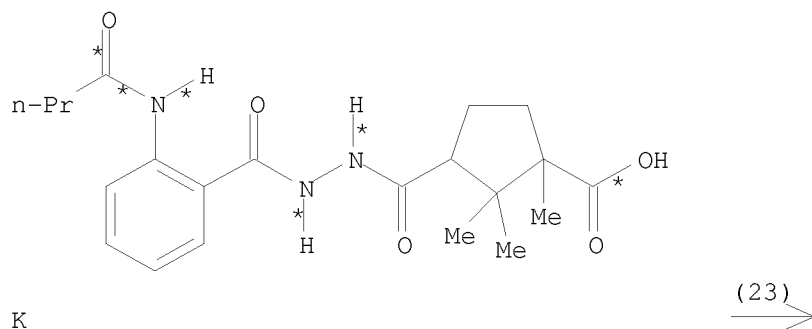
T  
YIELD 78%

RX(21)      RCT    I 860479-67-0  
             PRO    T 860479-75-0

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CON 45 minutes, 220 - 230 deg C  
NTE regioselective, thermal, alternative preparation shown, no  
solvent

RX(23) OF 64 ...K ==> U



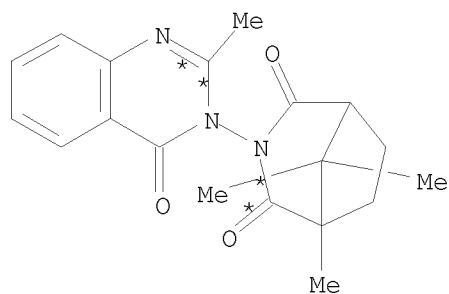
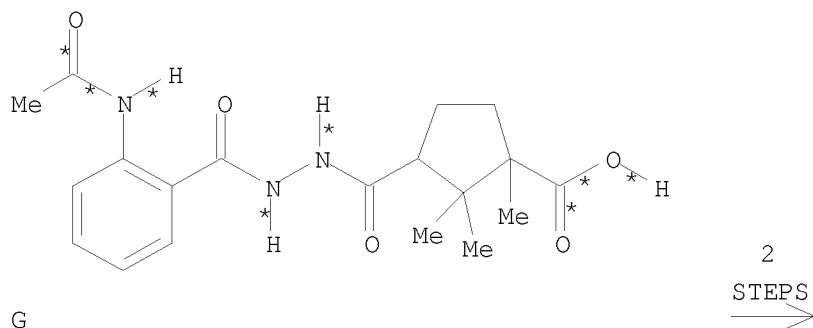
U  
YIELD 76%

RX(23) RCT K 860479-68-1  
PRO U 860479-76-1  
CON 45 minutes, 220 - 230 deg C  
NTE regioselective, thermal, alternative preparation shown, no  
solvent

RX(44) OF 64 COMPOSED OF RX(14), RX(18)  
RX(44) G ==> S



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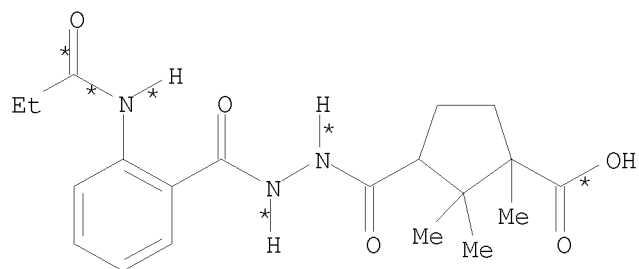
YIELD 89%

RX(14)     RCT   G 860479-66-9  
           RGT   V 68-12-2 DMF  
           PRO   N 860479-70-5  
           SOL   1330-20-7 Xylene  
           CON   15 - 20 minutes, reflux  
           NTE   regioselective, alternative preparation shown, brombenzene/agent  
                 gave similar results

RX(18)     RCT   N 860479-70-5  
           RGT   X 108-24-7 Ac2O  
           PRO   S 860479-74-9  
           SOL   64-19-7 AcOH  
           CON   40 minutes, heated  
           NTE   regioselective, alternative preparation shown

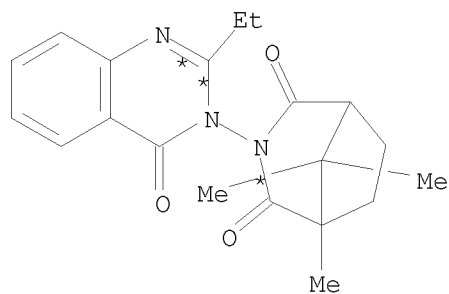
RX(46) OF 64 COMPOSED OF RX(15), RX(20)

RX(46)     I   ==>   T



I

2  
STEPS  
→

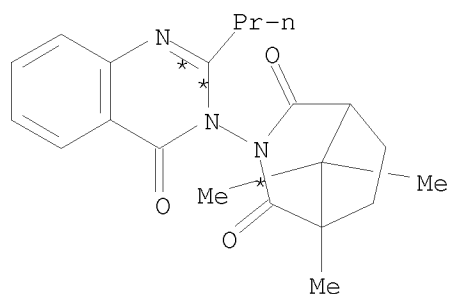
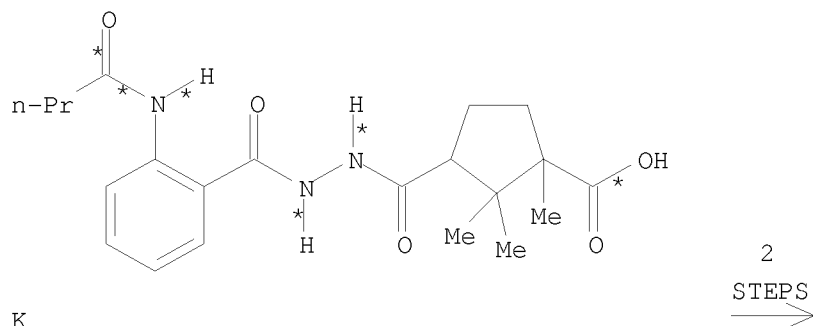


T

RX(15)     RCT   I 860479-67-0  
              RGT   V 68-12-2 DMF  
              PRO   P 860479-71-6  
              SOL   1330-20-7 Xylene  
              CON   15 - 20 minutes, reflux  
              NTE   regioselective, alternative preparation shown, brombenzene/agent  
                  gave similar results

RX(20)     RCT   P 860479-71-6  
              RGT   X 108-24-7 Ac2O  
              PRO   T 860479-75-0  
              SOL   64-19-7 AcOH  
              CON   40 minutes, heated  
              NTE   regioselective, alternative preparation shown

RX(48) OF 64 COMPOSED OF RX(16), RX(22)  
 RX(48)     K     ==>   U



RX(16)    RCT    K 860479-68-1  
           RGT    V 68-12-2 DMF  
           PRO    Q 860479-72-7  
           SOL    1330-20-7 Xylene  
           CON    SUBSTAGE(1) 15 - 20 minutes, reflux  
                   SUBSTAGE(2) cooled  
           NTE    regioselective, alternative preparation shown, brombenzene/agent  
                   gave similar results

RX(22)    RCT    Q 860479-72-7  
           RGT    X 108-24-7 Ac2O  
           PRO    U 860479-76-1  
           SOL    64-19-7 AcOH  
           CON    40 minutes, heated  
           NTE    regioselective, alternative preparation shown

L3    ANSWER 49 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER:    143:153337    CASREACT

TITLE:    Synthesis and structure-activity relationship of  
           3-phenyl-3H-quinazolin-4-one derivatives as CXCR3  
           chemokine receptor antagonists

AUTHOR(S):    Storelli, Stefania; Verdijk, Pauline; Verzijl, Dennis;  
                   Timmerman, Henk; van de Stolpe, Andrea C.; Tensen,  
                   Cornelis P.; Smit, Martine J.; De Esch, Iwan J. P.;

CORPORATE SOURCE: Leurs, Rob  
 Leiden/Amsterdam Center for Drug Research (LACDR),  
 Division of Medicinal Chemistry, Faculty of Sciences,  
 Vrije Universiteit Amsterdam, Amsterdam, 1081 HV,  
 Neth.

SOURCE: Bioorganic & Medicinal Chemistry Letters (2005),  
 15(11), 2910-2913  
 CODEN: BMCLE8; ISSN: 0960-894X

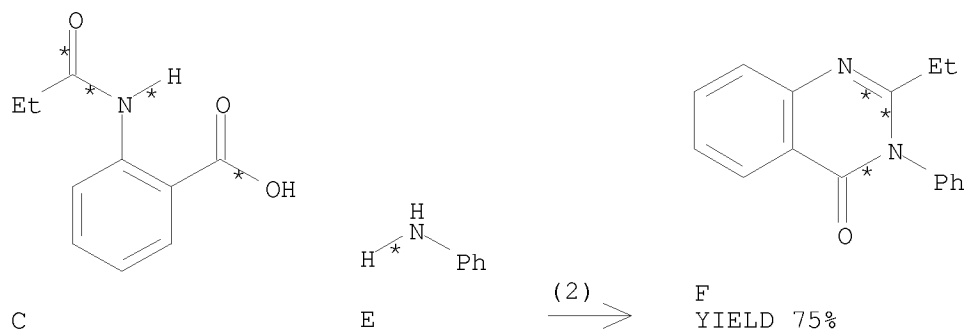
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

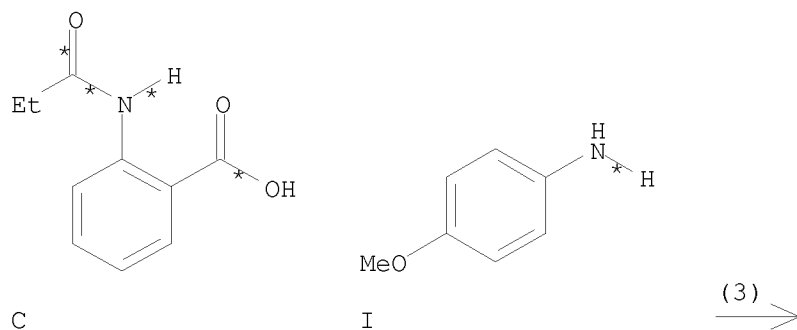
AB A series of 3-phenyl-3H-quinazolin-4-ones have been synthesized and tested for affinity and activity at the chemokine CXCR3 receptor. The most potent compound has been evaluated using radioligand binding and calcium mobilization assays and is considered a useful tool for further characterization of the CXCR3 receptor.

RX(2) OF 173 ...C + E ==&gt; F...

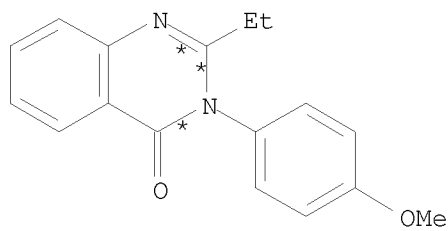


RX(2) RCT C 19165-26-5, E 62-53-3  
 RGT G 7719-12-2 PC13  
 PRO F 5260-41-3  
 SOL 108-88-3 PhMe

RX(3) OF 173 ...C + I ==&gt; J...

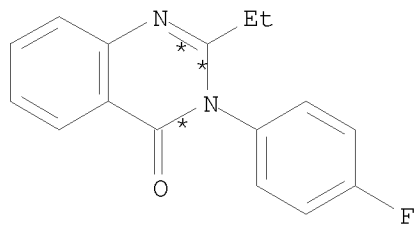
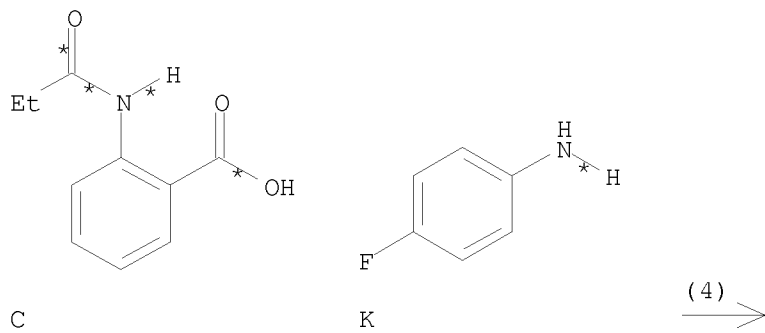


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J  
YIELD 75%

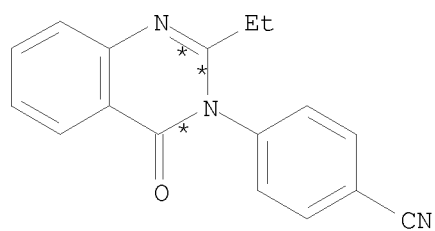
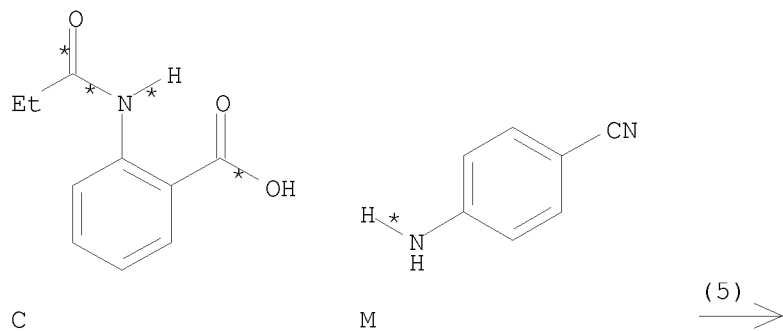
RX(3)      RCT   C 19165-26-5, I 104-94-9  
              RGT   G 7719-12-2 PC13  
              PRO   J 50498-62-9  
              SOL   108-88-3 PhMe

$$\text{RX}(4) \text{ OF } 173 \quad \dots \text{C} + \text{K} \implies \text{L} \dots$$


L  
YIELD 75%

RX(4)	RCT	C 19165-26-5, K 371-40-4
	RGT	G 7719-12-2 PC13
	PRO	L 329190-48-9
	SOL	108-88-3 PhMe

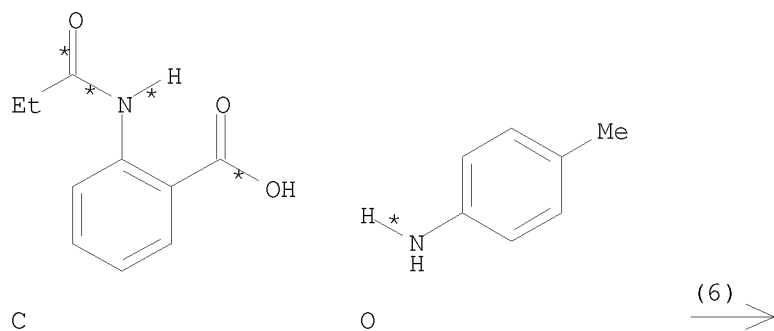
$$\text{RX}(5) \text{ OF } 173 \quad \dots \text{C} + \text{M} \implies \text{N} \dots$$



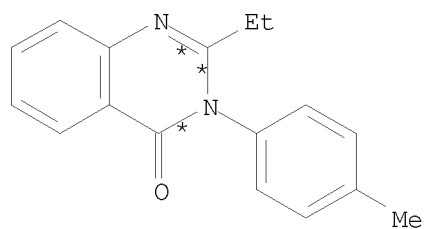
N  
YIELD 75%

RX(5)      RCT    C 19165-26-5, M 873-74-5  
              RGT    G 7719-12-2 PC13  
              PRO    N 860002-79-5  
              SOL    108-88-3 PhMe

RX(6) OF 173      ...C + O ==> P...



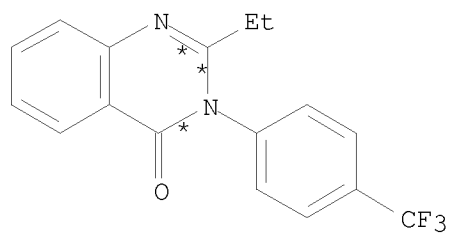
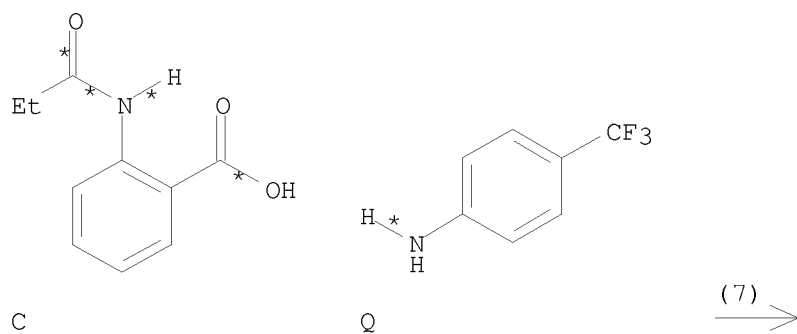
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P  
YIELD 75%

RX(6) RCT C 19165-26-5, O 106-49-0  
RGT G 7719-12-2 PC13  
PRO P 50498-61-8  
SOL 108-88-3 PhMe

RX(7) OF 173 ...C + Q ==> R...

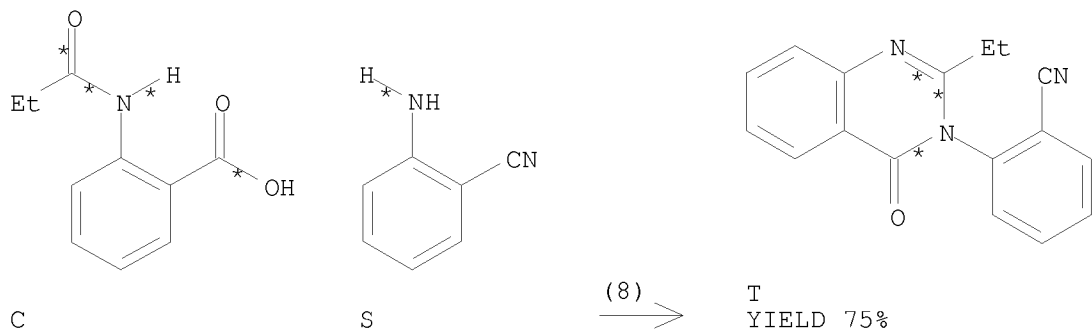


R  
YIELD 75%

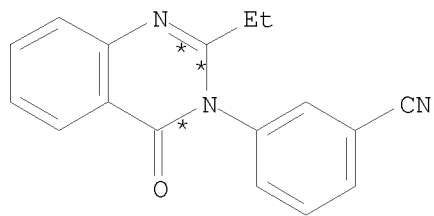
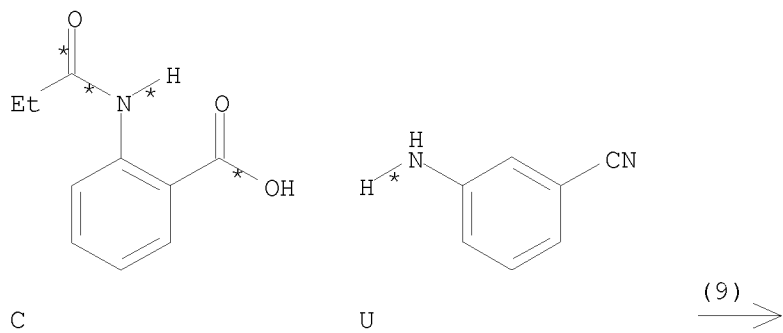
RX(7) RCT C 19165-26-5, Q 455-14-1  
RGT G 7719-12-2 PC13  
PRO R 860002-80-8  
SOL 108-88-3 PhMe

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RX(8) OF 173            ...C + S ==> T...



RX(8)	RCT	C 19165-26-5, S 1885-29-6
	RGT	G 7719-12-2 PC13
	PRO	T 860002-81-9
	SOL	108-88-3 PhMe

$$\text{RX(9) OF 173} \quad \dots \text{C} + \text{U} \implies \text{V} \dots$$


V  
YIELD 75%

RX(9)            RCT   C 19165-26-5, U 2237-30-1  
                  RGT   G 7719-12-2 PC13  
                  PRO   V 860002-82-0

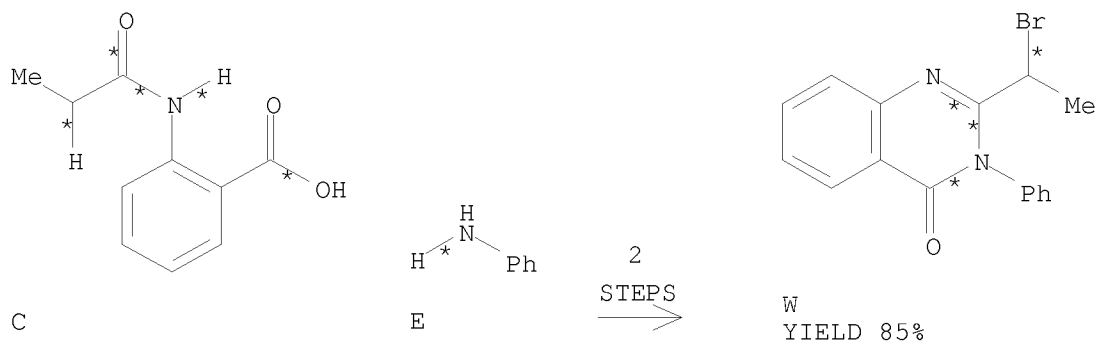


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SOL 108-88-3 PhMe

RX(49) OF 173 COMPOSED OF RX(2), RX(10)

RX(49) C + E ==> W



RX(2) RCT C 19165-26-5, E 62-53-3

RGT G 7719-12-2 PC13

PRO F 5260-41-3

SOL 108-88-3 PhMe

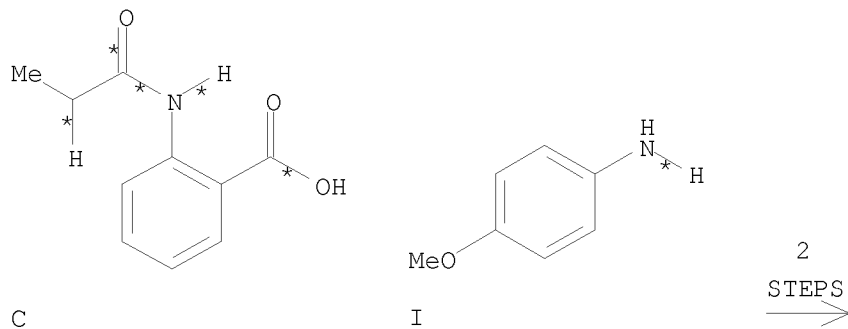
RX(10) RCT F 5260-41-3

RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br<sub>2</sub>

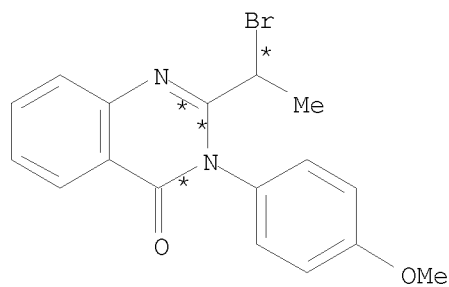
PRO W 860002-83-1

RX(50) OF 173 COMPOSED OF RX(3), RX(11)

RX(50) C + I ==> AA



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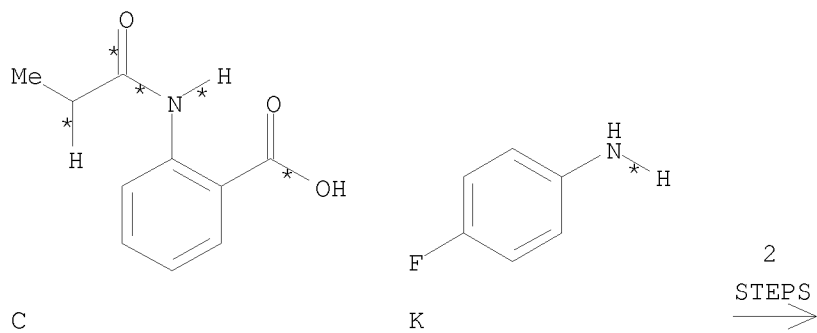


AA  
YIELD 85%

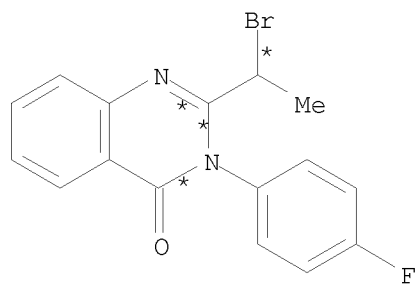
RX(3)        RCT    C 19165-26-5, I 104-94-9  
              RGT    G 7719-12-2 PC13  
              PRO    J 50498-62-9  
              SOL    108-88-3 PhMe

RX(11)       RCT    J 50498-62-9  
              RGT    X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
              PRO    AA 473721-15-2

RX(51) OF 173 COMPOSED OF RX(4), RX(12)  
RX(51)       C    +    K    ==>    AB



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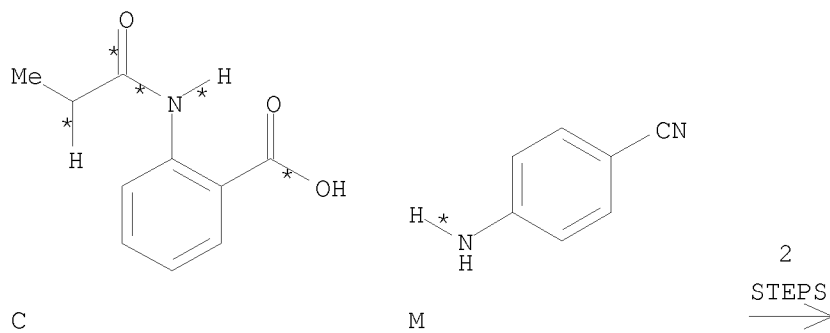


AB  
YIELD 85%

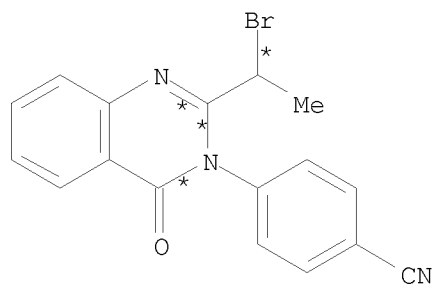
RX(4)        RCT    C 19165-26-5, K 371-40-4  
              RGT    G 7719-12-2 PC13  
              PRO    L 329190-48-9  
              SOL    108-88-3 PhMe

RX(12)       RCT    L 329190-48-9  
              RGT    X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
              PRO    AB 329190-49-0

RX(52) OF 173 COMPOSED OF RX(5), RX(13)  
RX(52)       C    +    M    ==>    AC



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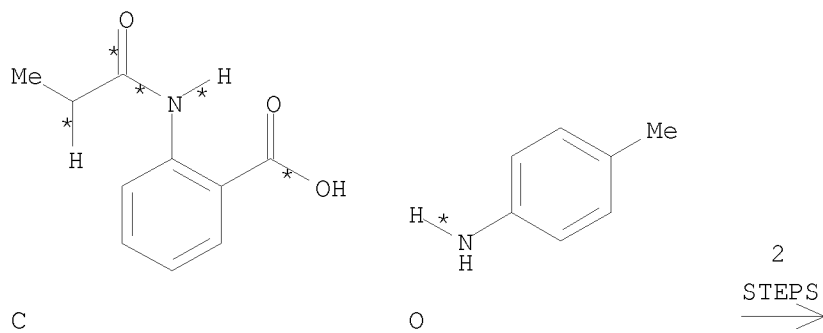


AC  
YIELD 85%

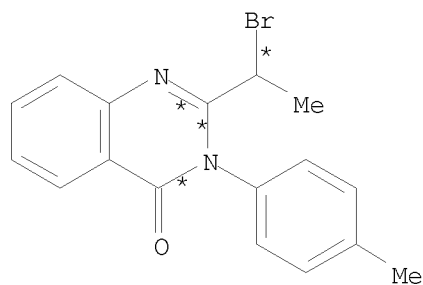
RX(5)        RCT    C 19165-26-5, M 873-74-5  
              RGT    G 7719-12-2 PC13  
              PRO    N 860002-79-5  
              SOL    108-88-3 PhMe

RX(13)       RCT    N 860002-79-5  
              RGT    X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
              PRO    AC 860002-84-2

RX(53) OF 173 COMPOSED OF RX(6), RX(14)  
RX(53)       C    +    O    ==>    AD



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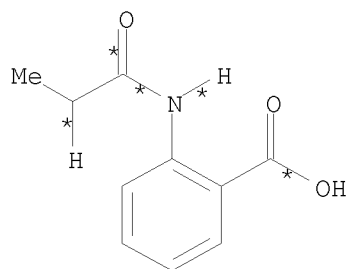
AD  
YIELD 85%

RX(6) RCT C 19165-26-5, O 106-49-0  
RGT G 7719-12-2 PC13  
PRO P 50498-61-8  
SOL 108-88-3 PhMe

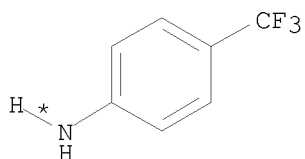
RX(14) RCT P 50498-61-8  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AD 860002-85-3

RX(54) OF 173 COMPOSED OF RX(7), RX(15)

RX(54) C + Q ==> AE



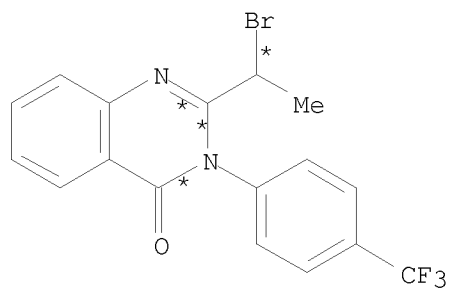
C



Q

2  
STEPS  
→

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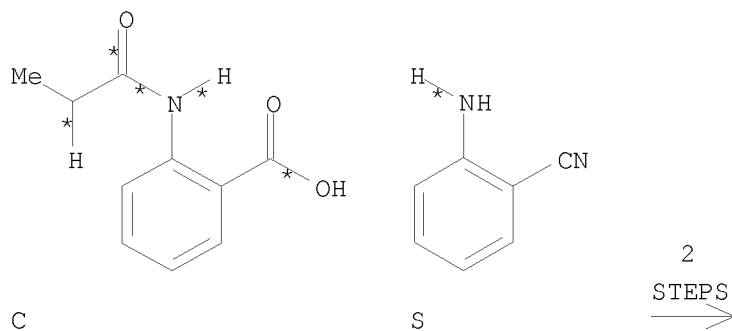


AE  
YIELD 85%

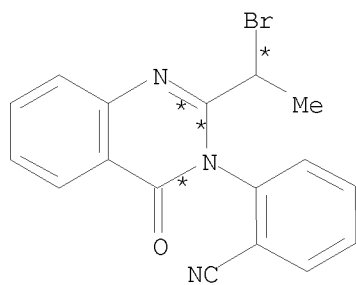
RX(7)        RCT    C 19165-26-5, Q 455-14-1  
              RGT    G 7719-12-2 PC13  
              PRO    R 860002-80-8  
              SOL    108-88-3 PhMe

RX(15)       RCT    R 860002-80-8  
              RGT    X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
              PRO    AE 860002-86-4

RX(55) OF 173 COMPOSED OF RX(8), RX(16)  
RX(55)       C    +    S    ==>    AF



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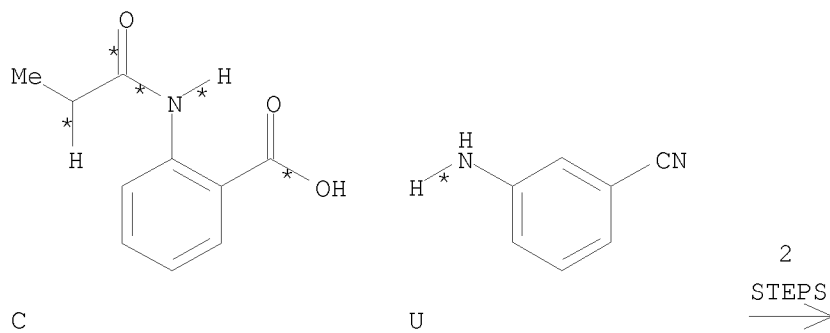


AF  
YIELD 85%

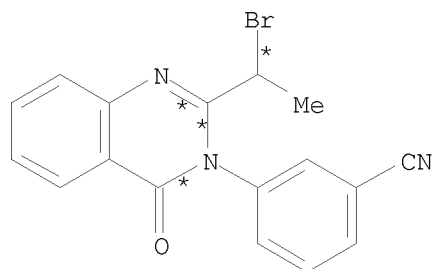
RX(8)        RCT    C 19165-26-5, S 1885-29-6  
              RGT    G 7719-12-2 PC13  
              PRO    T 860002-81-9  
              SOL    108-88-3 PhMe

RX(16)       RCT    T 860002-81-9  
              RGT    X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
              PRO    AF 860002-87-5

RX(56) OF 173 COMPOSED OF RX(9), RX(17)  
RX(56)       C    +    U    ==>    AG



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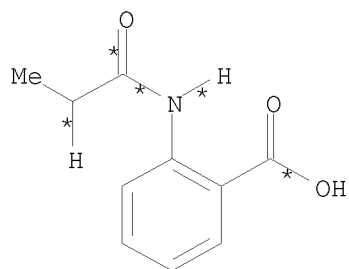


AG  
YIELD 85%

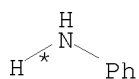
RX(9)        RCT    C 19165-26-5, U 2237-30-1  
              RGT    G 7719-12-2 PC13  
              PRO    V 860002-82-0  
              SOL    108-88-3 PhMe

RX(17)       RCT    V 860002-82-0  
              RGT    X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
              PRO    AG 860002-88-6

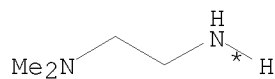
RX(89) OF 173 COMPOSED OF RX(2), RX(10), RX(18)  
RX(89)       C    +    E    +    AH    ==>    AI



C



E

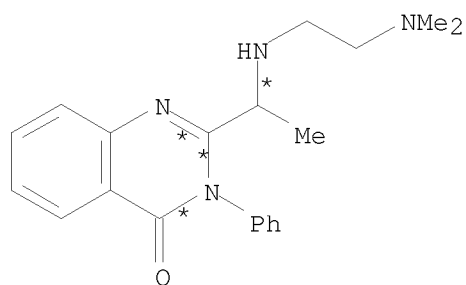


AH

3  
STEPS  
→



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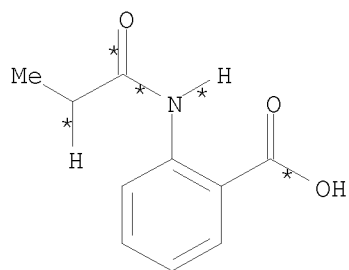
AI  
YIELD 65%

RX(2) RCT C 19165-26-5, E 62-53-3  
RGT G 7719-12-2 PC13  
PRO F 5260-41-3  
SOL 108-88-3 PhMe

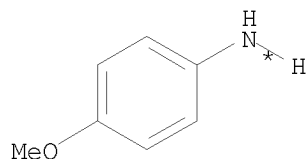
RX(10) RCT F 5260-41-3  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO W 860002-83-1

RX(18) RCT W 860002-83-1, AH 108-00-9  
PRO AI 860002-89-7  
SOL 64-17-5 EtOH  
CON reflux

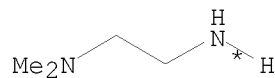
RX(91) OF 173 COMPOSED OF RX(3), RX(11), RX(19)  
RX(91) C + I + AH ==> AK



C



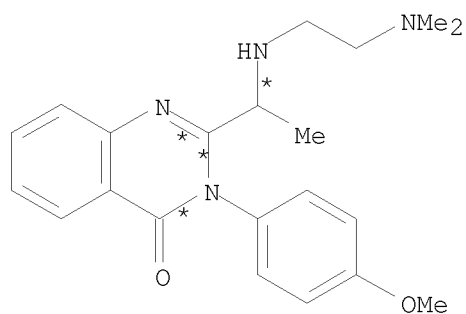
I



AH

3  
STEPS  
→

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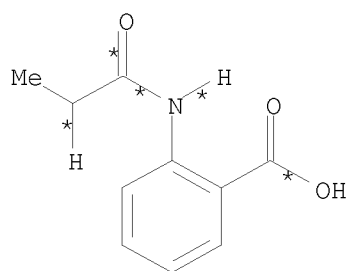
AK  
YIELD 65%

RX(3) RCT C 19165-26-5, I 104-94-9  
RGT G 7719-12-2 PC13  
PRO J 50498-62-9  
SOL 108-88-3 PhMe

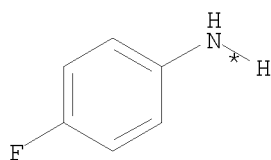
RX(11) RCT J 50498-62-9  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AA 473721-15-2

RX(19) RCT AA 473721-15-2, AH 108-00-9  
PRO AK 473721-16-3  
SOL 64-17-5 EtOH  
CON reflux

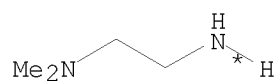
RX(93) OF 173 COMPOSED OF RX(4), RX(12), RX(20)  
RX(93) C + K + AH ==> AL



C



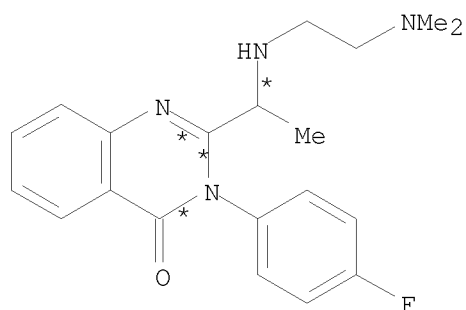
K



AH

3  
STEPS  
=>

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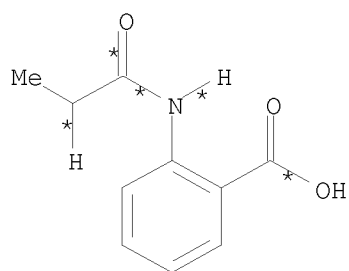
AL  
YIELD 65%

RX(4) RCT C 19165-26-5, K 371-40-4  
RGT G 7719-12-2 PC13  
PRO L 329190-48-9  
SOL 108-88-3 PhMe

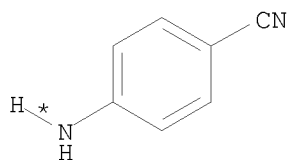
RX(12) RCT L 329190-48-9  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AB 329190-49-0

RX(20) RCT AB 329190-49-0, AH 108-00-9  
PRO AL 329190-50-3  
SOL 64-17-5 EtOH  
CON reflux

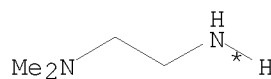
RX(95) OF 173 COMPOSED OF RX(5), RX(13), RX(21)  
RX(95) C + M + AH ==> AM



C



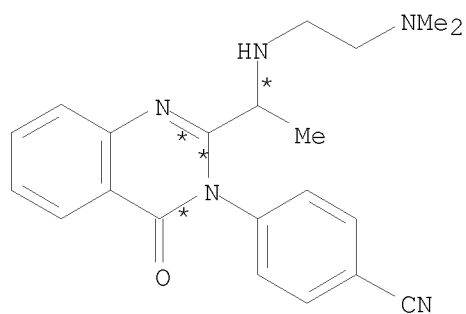
M



AH

3  
STEPS  
=>

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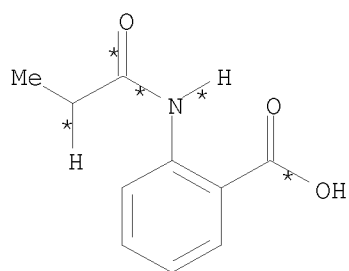
AM  
YIELD 65%

RX(5) RCT C 19165-26-5, M 873-74-5  
RGT G 7719-12-2 PC13  
PRO N 860002-79-5  
SOL 108-88-3 PhMe

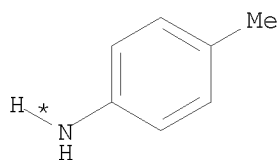
RX(13) RCT N 860002-79-5  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AC 860002-84-2

RX(21) RCT AC 860002-84-2, AH 108-00-9  
PRO AM 860002-90-0  
SOL 64-17-5 EtOH  
CON reflux

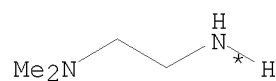
RX(97) OF 173 COMPOSED OF RX(6), RX(14), RX(22)  
RX(97) C + O + AH ==> AN



C



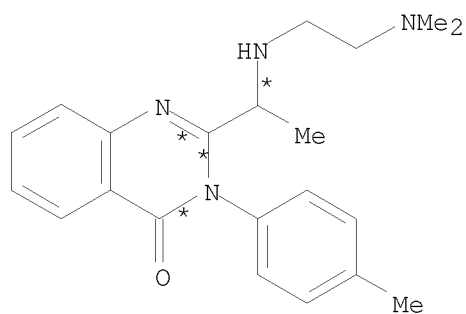
O



AH

3  
STEPS  
=>

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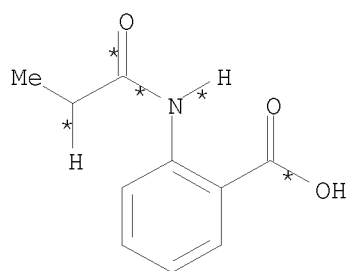
AN  
YIELD 65%

RX(6) RCT C 19165-26-5, O 106-49-0  
RGT G 7719-12-2 PC13  
PRO P 50498-61-8  
SOL 108-88-3 PhMe

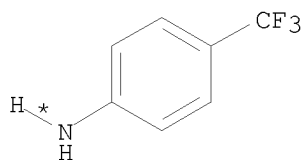
RX(14) RCT P 50498-61-8  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AD 860002-85-3

RX(22) RCT AD 860002-85-3, AH 108-00-9  
PRO AN 854622-82-5  
SOL 64-17-5 EtOH  
CON reflux

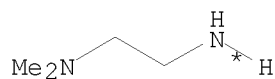
RX(99) OF 173 COMPOSED OF RX(7), RX(15), RX(23)  
RX(99) C + Q + AH ==> AO



C



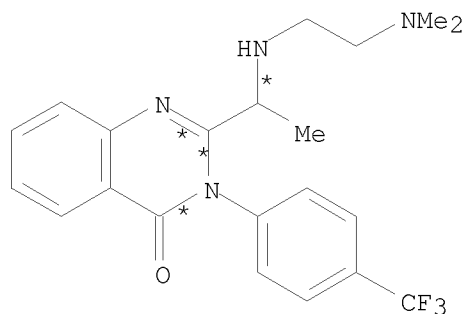
Q



AH

3  
STEPS  
=>

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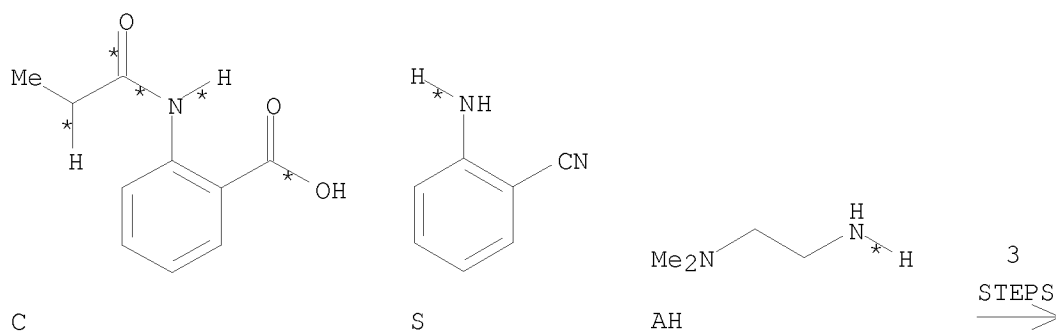
AO  
YIELD 65%

RX(7) RCT C 19165-26-5, Q 455-14-1  
RGT G 7719-12-2 PC13  
PRO R 860002-80-8  
SOL 108-88-3 PhMe

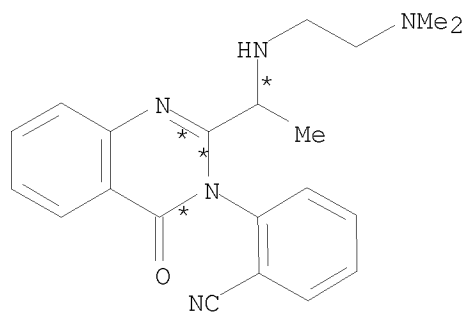
RX(15) RCT R 860002-80-8  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AE 860002-86-4

RX(23) RCT AE 860002-86-4, AH 108-00-9  
PRO AO 860002-91-1  
SOL 64-17-5 EtOH  
CON reflux

RX(101) OF 173 COMPOSED OF RX(8), RX(16), RX(24)  
RX(101) C + S + AH ==> AP



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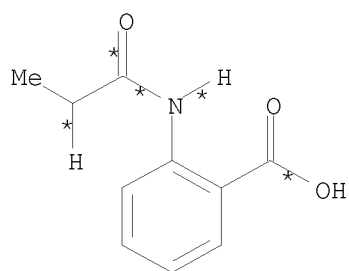
AP  
YIELD 65%

RX(8)        RCT    C 19165-26-5, S 1885-29-6  
              RGT    G 7719-12-2 PC13  
              PRO    T 860002-81-9  
              SOL    108-88-3 PhMe

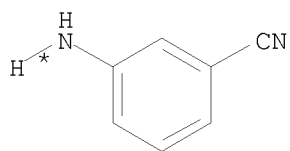
RX(16)       RCT    T 860002-81-9  
              RGT    X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
              PRO    AF 860002-87-5

RX(24)       RCT    AF 860002-87-5, AH 108-00-9  
              PRO    AP 860002-92-2  
              SOL    64-17-5 EtOH  
              CON    reflux

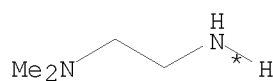
RX(103) OF 173 COMPOSED OF RX(9), RX(17), RX(25)  
RX(103)    C   +   U   +   AH   ==>   AQ



C



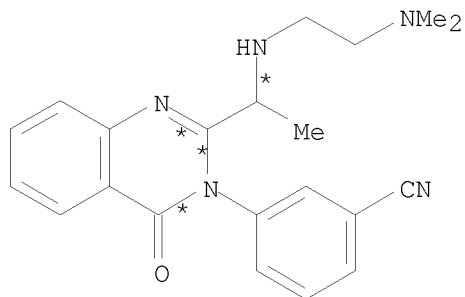
U



AH

3  
STEPS  
=>

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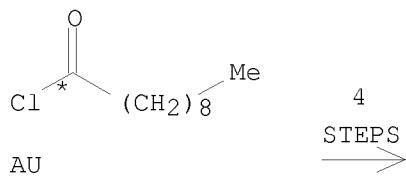
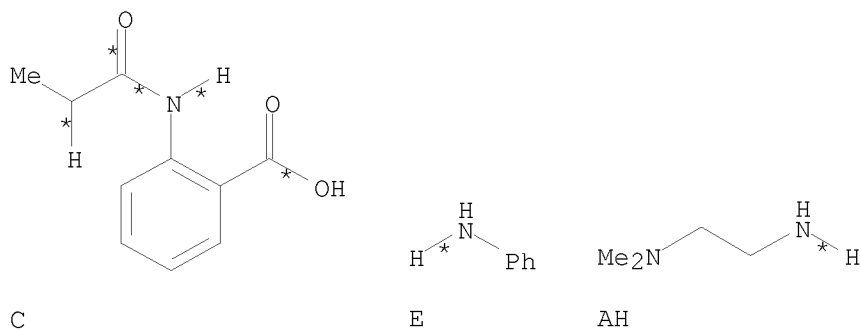
AQ  
YIELD 65%

RX(9)	RCT	C 19165-26-5, U 2237-30-1
	RGT	G 7719-12-2 PC13
	PRO	V 860002-82-0
	SOL	108-88-3 PhMe

RX(17) RCT V 860002-82-0  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AG 860002-88-6

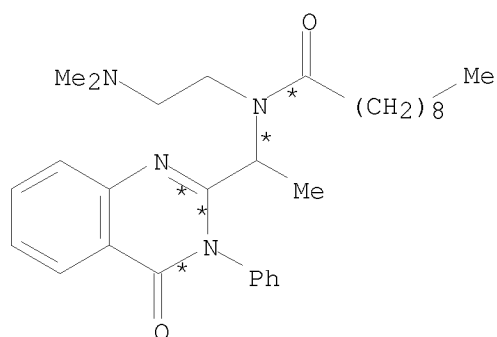
RX(25) RCT AG 860002-88-6, AH 108-00-9  
PRO AQ 860002-93-3  
SOL 64-17-5 EtOH  
CON reflux

RX(106) OF 173 COMPOSED OF RX(2), RX(10), RX(18), RX(27)  
 RX(106) C + E + AH + AU ==> AV





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AV  
YIELD 55%

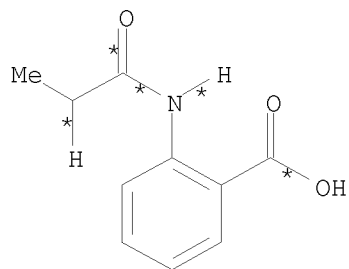
RX(2) RCT C 19165-26-5, E 62-53-3  
RGT G 7719-12-2 PC13  
PRO F 5260-41-3  
SOL 108-88-3 PhMe

RX(10) RCT F 5260-41-3  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br<sub>2</sub>  
PRO W 860002-83-1

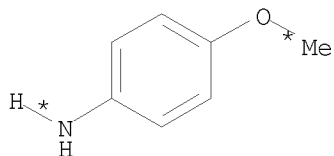
RX(18) RCT W 860002-83-1, AH 108-00-9  
PRO AI 860002-89-7  
SOL 64-17-5 EtOH  
CON reflux

RX(27) RCT AI 860002-89-7, AU 112-13-0  
RGT AW 121-44-8 Et<sub>3</sub>N  
PRO AV 334516-31-3  
SOL 123-91-1 Dioxane

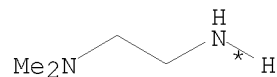
RX(109) OF 173 COMPOSED OF RX(3), RX(11), RX(19), RX(26)  
RX(109) C + I + AH ==> AR



C



I

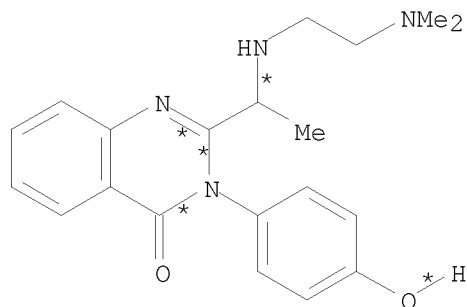


AH

4

STEPS  
→

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AR  
YIELD 15%

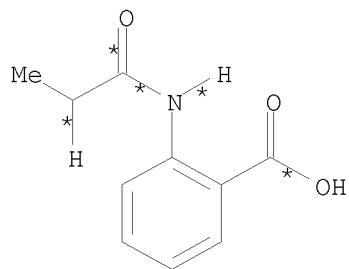
RX(3) RCT C 19165-26-5, I 104-94-9  
RGT G 7719-12-2 PC13  
PRO J 50498-62-9  
SOL 108-88-3 PhMe

RX(11) RCT J 50498-62-9  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AA 473721-15-2

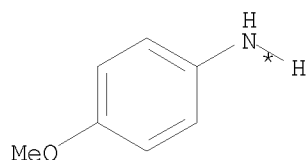
RX(19) RCT AA 473721-15-2, AH 108-00-9  
PRO AK 473721-16-3  
SOL 64-17-5 EtOH  
CON reflux

RX(26) RCT AK 473721-16-3  
RGT AS 10294-33-4 BBr3  
PRO AR 860002-94-4  
SOL 67-56-1 MeOH

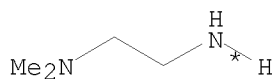
RX(110) OF 173 COMPOSED OF RX(3), RX(11), RX(19), RX(28)  
RX(110) C + I + AH + AU ==> AY



C

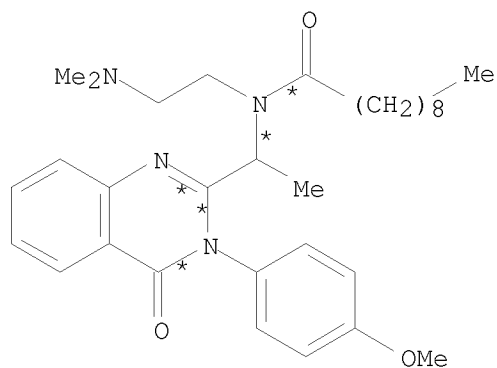
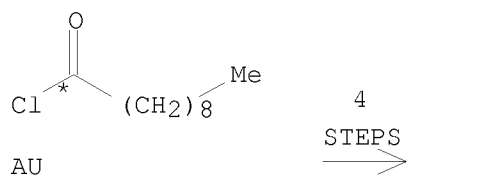


I



AH

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AY  
YIELD 55%

RX(3) RCT C 19165-26-5, I 104-94-9  
RGT G 7719-12-2 PC13  
PRO J 50498-62-9  
SOL 108-88-3 PhMe

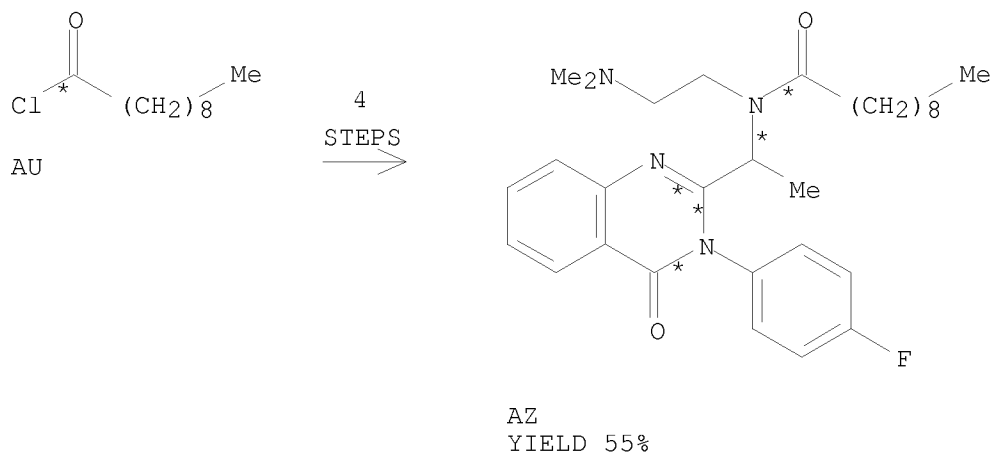
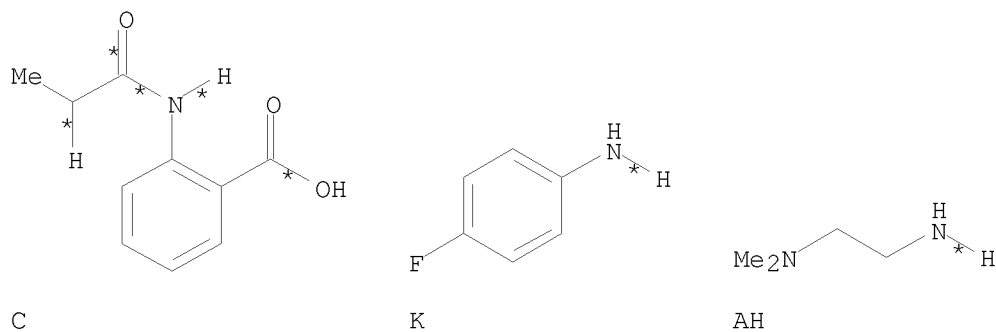
RX(11) RCT J 50498-62-9  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AA 473721-15-2

RX(19) RCT AA 473721-15-2, AH 108-00-9  
PRO AK 473721-16-3  
SOL 64-17-5 EtOH  
CON reflux

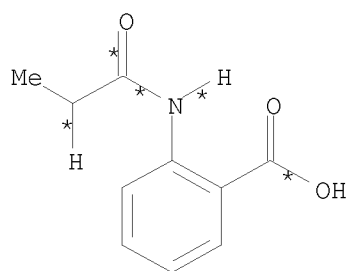
RX(28) RCT AK 473721-16-3, AU 112-13-0  
RGT AW 121-44-8 Et3N  
PRO AY 329190-30-9  
SOL 123-91-1 Dioxane

RX(116) OF 173 COMPOSED OF RX(4), RX(12), RX(20), RX(29)  
RX(116) C + K + AH + AU ==> AZ

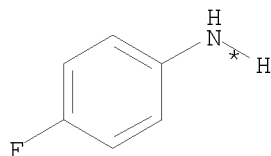
10/ 562,112



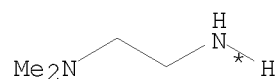
RX(4)	RCT	C 19165-26-5, K 371-40-4
	RGT	G 7719-12-2 PC13
	PRO	L 329190-48-9
	SOL	108-88-3 PhMe
RX(12)	RCT	L 329190-48-9
	RGT	X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
	PRO	AB 329190-49-0
RX(20)	RCT	AB 329190-49-0, AH 108-00-9
	PRO	AL 329190-50-3
	SOL	64-17-5 EtOH
	CON	reflux
RX(29)	RCT	AL 329190-50-3, AU 112-13-0
	RGT	AW 121-44-8 Et3N
	PRO	AZ 329190-29-6
	SOL	123-91-1 Dioxane
RX(117) OF 173 COMPOSED OF RX(4), RX(12), RX(20), RX(35)		
RX(117)	C + K + AH + AY + BF ==> BG + BH	



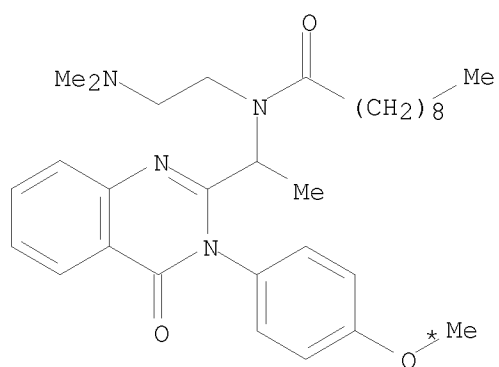
C



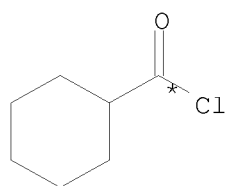
K



AH

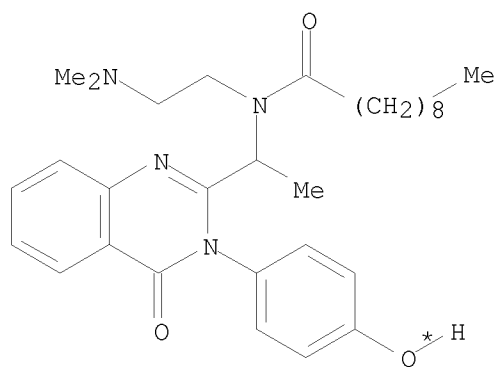


AY

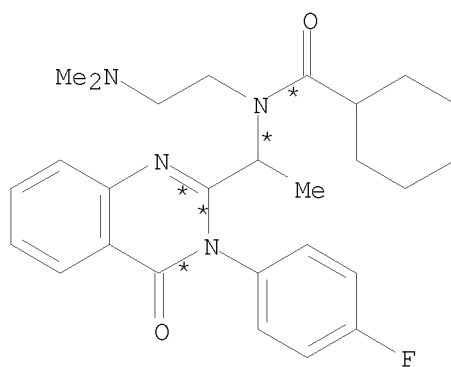


BF

4  
STEPS  
→



BG  
YIELD 15%



BH  
YIELD 55%

RX(4) RCT C 19165-26-5, K 371-40-4  
RGT G 7719-12-2 PC13  
PRO L 329190-48-9  
SOL 108-88-3 PhMe

RX(12) RCT L 329190-48-9

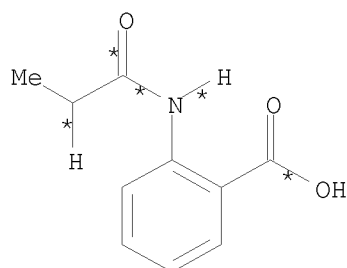
10/ 562,112

RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AB 329190-49-0

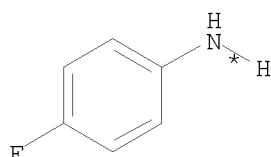
RX(20) RCT AB 329190-49-0, AH 108-00-9  
PRO AL 329190-50-3  
SOL 64-17-5 EtOH  
CON reflux

RX(35) RCT AL 329190-50-3, AY 329190-30-9, BF 2719-27-9  
RGT AW 121-44-8 Et3N, AS 10294-33-4 BBr3  
PRO BG 860002-99-9, BH 860003-00-5  
SOL 67-56-1 MeOH, 123-91-1 Dioxane

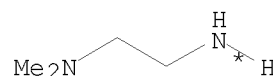
RX(118) OF 173 COMPOSED OF RX(4), RX(12), RX(20), RX(36)  
RX(118) C + K + AH + BF ==> BH



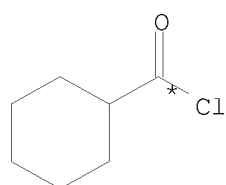
C



K

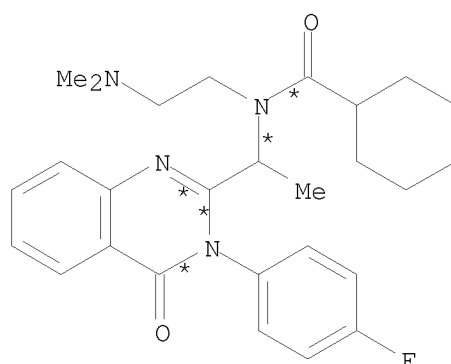


AH



BF

4  
STEPS  
➔



BH  
YIELD 55%

RX(4) RCT C 19165-26-5, K 371-40-4  
RGT G 7719-12-2 PCl3  
PRO L 329190-48-9  
SOL 108-88-3 PhMe

RX(12) RCT L 329190-48-9  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2

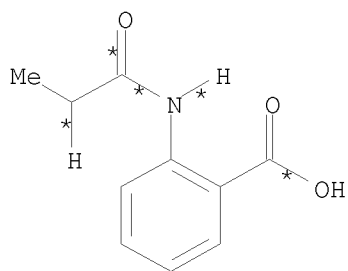
10/ 562,112

PRO AB 329190-49-0

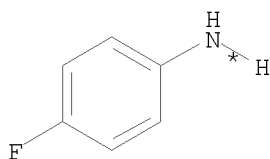
RX(20) RCT AB 329190-49-0, AH 108-00-9  
PRO AL 329190-50-3  
SOL 64-17-5 EtOH  
CON reflux

RX(36) RCT AL 329190-50-3, BF 2719-27-9  
RGT AW 121-44-8 Et3N  
PRO BH 860003-00-5  
SOL 123-91-1 Dioxane

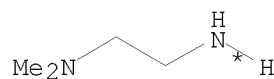
RX(119) OF 173 COMPOSED OF RX(4), RX(12), RX(20), RX(38)  
RX(119) C + K + AH + BJ ==> BK



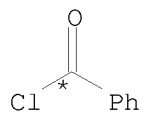
C



K

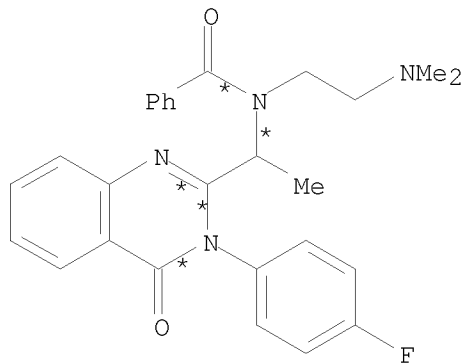


AH



BJ

4  
STEPS  
→



BK  
YIELD 55%

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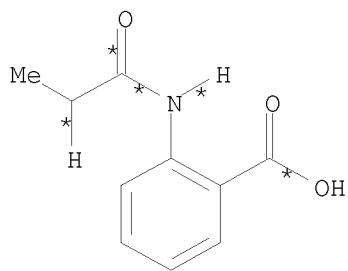
RX(4) RCT C 19165-26-5, K 371-40-4  
RGT G 7719-12-2 PC13  
PRO L 329190-48-9  
SOL 108-88-3 PhMe

RX(12) RCT L 329190-48-9  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AB 329190-49-0

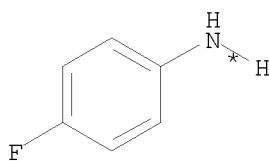
RX(20) RCT AB 329190-49-0, AH 108-00-9  
PRO AL 329190-50-3  
SOL 64-17-5 EtOH  
CON reflux

RX(38) RCT AL 329190-50-3, BJ 98-88-4  
RGT AW 121-44-8 Et3N  
PRO BK 860003-02-7  
SOL 123-91-1 Dioxane

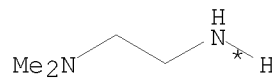
RX(120) OF 173 COMPOSED OF RX(4), RX(12), RX(20), RX(40)  
RX(120) C + K + AH + BM ==> BN



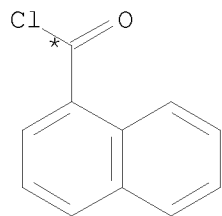
C



K

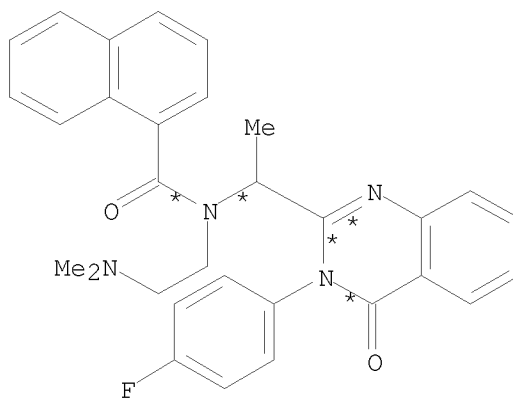


AH



BM

4  
STEPS  
→



BN  
YIELD 55%

RX(4) RCT C 19165-26-5, K 371-40-4



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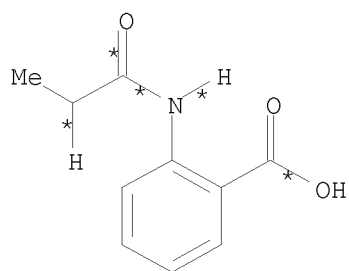
RGT G 7719-12-2 PC13  
PRO L 329190-48-9  
SOL 108-88-3 PhMe

RX(12) RCT L 329190-48-9  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AB 329190-49-0

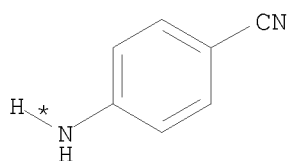
RX(20) RCT AB 329190-49-0, AH 108-00-9  
PRO AL 329190-50-3  
SOL 64-17-5 EtOH  
CON reflux

RX(40) RCT AL 329190-50-3, BM 879-18-5  
RGT AW 121-44-8 Et3N  
PRO BN 334904-56-2  
SOL 123-91-1 Dioxane

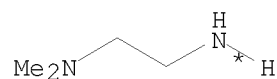
RX(124) OF 173 COMPOSED OF RX(5), RX(13), RX(21), RX(30)  
RX(124) C + M + AH + AU ==> BA



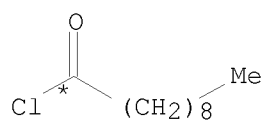
C



M



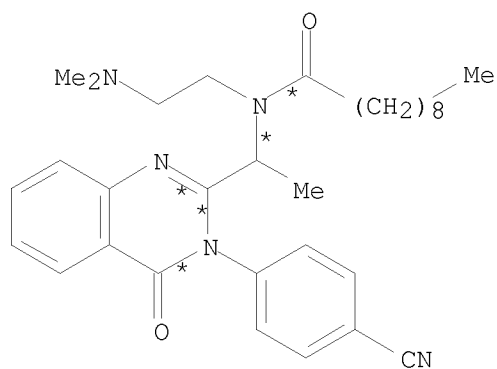
AH



AU

4  
STEPS  
→

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BA  
YIELD 55%

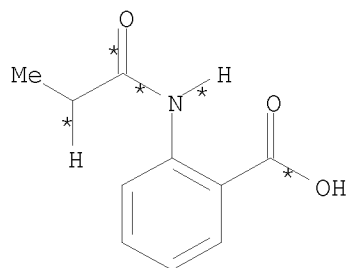
RX(5) RCT C 19165-26-5, M 873-74-5  
RGT G 7719-12-2 PC13  
PRO N 860002-79-5  
SOL 108-88-3 PhMe

RX(13) RCT N 860002-79-5  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br<sub>2</sub>  
PRO AC 860002-84-2

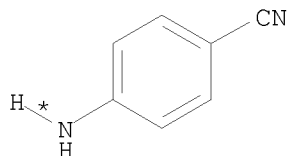
RX(21) RCT AC 860002-84-2, AH 108-00-9  
PRO AM 860002-90-0  
SOL 64-17-5 EtOH  
CON reflux

RX(30) RCT AM 860002-90-0, AU 112-13-0  
RGT AW 121-44-8 Et<sub>3</sub>N  
PRO BA 860002-95-5  
SOL 123-91-1 Dioxane

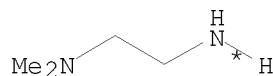
RX(125) OF 173 COMPOSED OF RX(5), RX(13), RX(21), RX(37)  
RX(125) C + M + AH + BF ==> BI



C

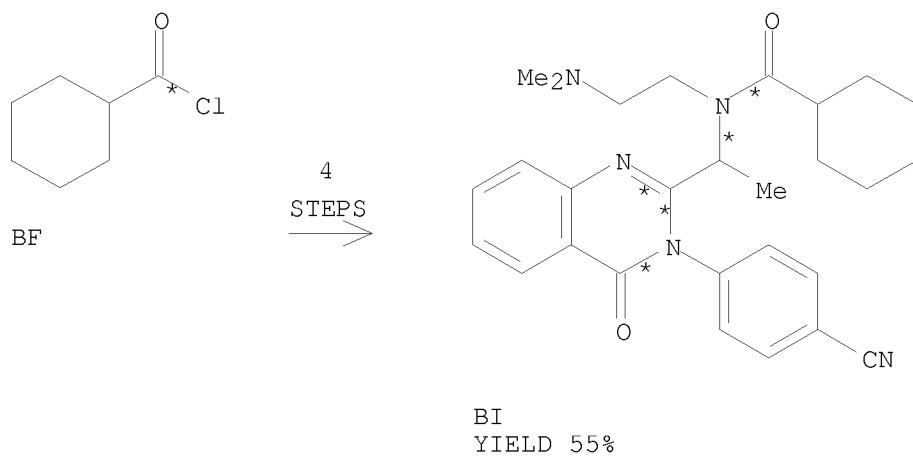


M



AH

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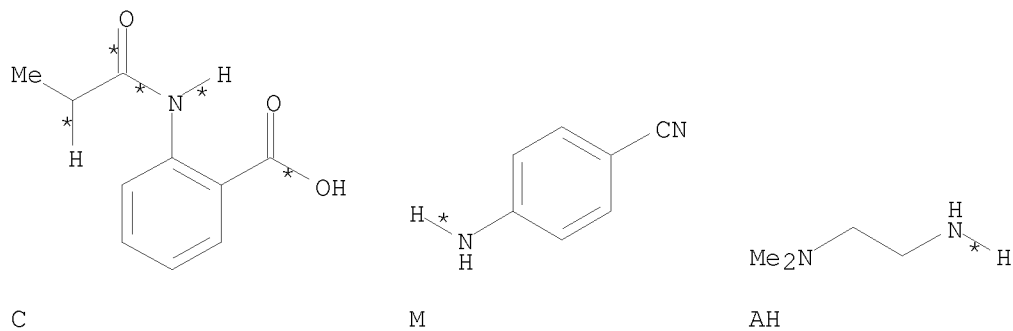
RX(5) RCT C 19165-26-5, M 873-74-5  
 RGT G 7719-12-2 PC13  
 PRO N 860002-79-5  
 SOL 108-88-3 PhMe

RX(13) RCT N 860002-79-5  
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
 PRO AC 860002-84-2

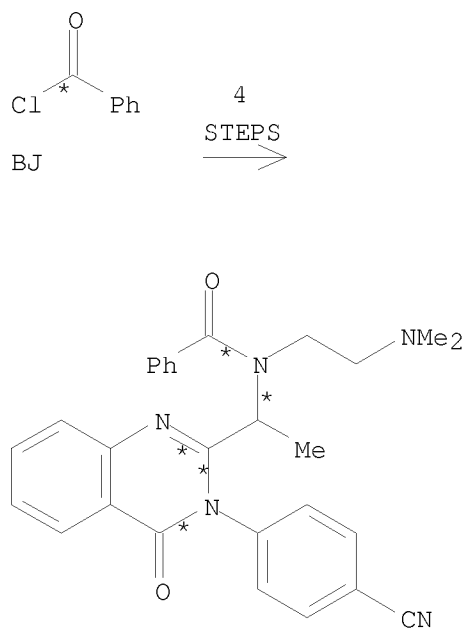
RX(21) RCT AC 860002-84-2, AH 108-00-9  
 PRO AM 860002-90-0  
 SOL 64-17-5 EtOH  
 CON reflux

RX(37) RCT AM 860002-90-0, BF 2719-27-9  
 RGT AW 121-44-8 Et3N  
 PRO BI 860003-01-6  
 SOL 123-91-1 Dioxane

RX(126) OF 173 COMPOSED OF RX(5), RX(13), RX(21), RX(39)  
 RX(126) C + M + AH + BJ ==> BL



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BL  
YIELD 55%

RX(5) RCT C 19165-26-5, M 873-74-5  
RGT G 7719-12-2 PC13  
PRO N 860002-79-5  
SOL 108-88-3 PhMe

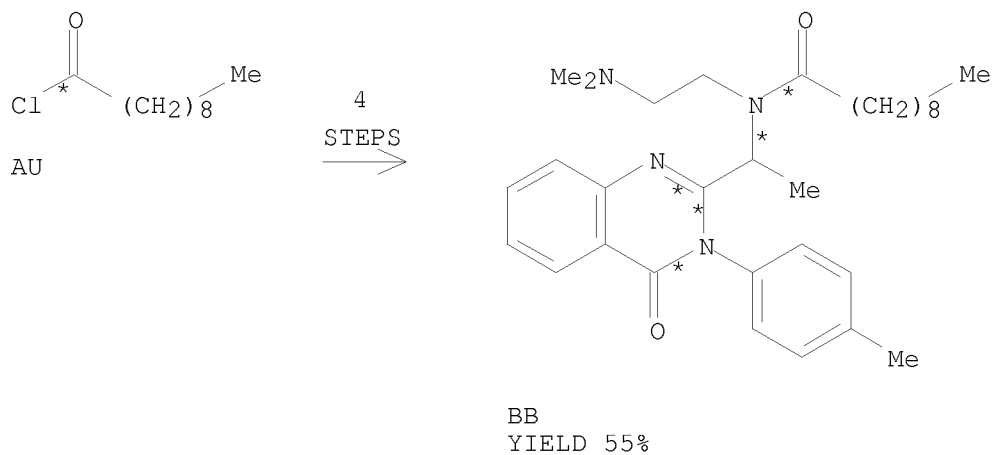
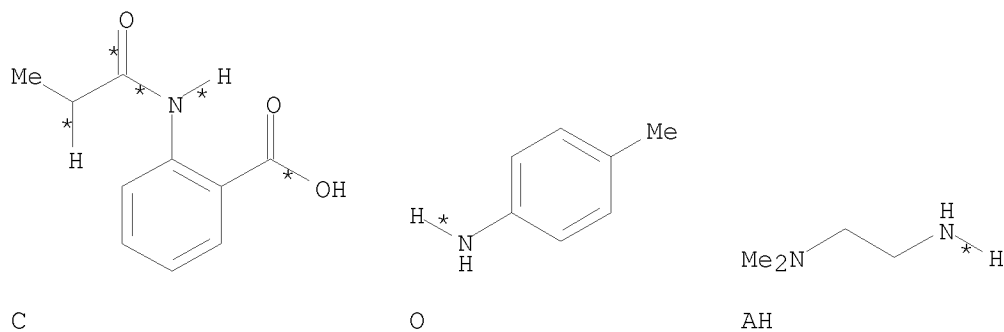
RX(13) RCT N 860002-79-5  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br<sub>2</sub>  
PRO AC 860002-84-2

RX(21) RCT AC 860002-84-2, AH 108-00-9  
PRO AM 860002-90-0  
SOL 64-17-5 EtOH  
CON reflux

RX(39) RCT AM 860002-90-0, BJ 98-88-4  
RGT AW 121-44-8 Et<sub>3</sub>N  
PRO BL 860003-03-8  
SOL 123-91-1 Dioxane

RX(128) OF 173 COMPOSED OF RX(6), RX(14), RX(22), RX(31)  
RX(128) C + O + AH + AU ==> BB

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RX(6) RCT C 19165-26-5, O 106-49-0  
RGT G 7719-12-2 PC13  
PRO P 50498-61-8  
SOL 108-88-3 PhMe

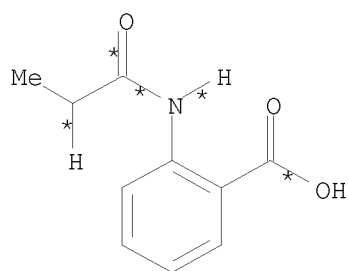
RX(14) RCT P 50498-61-8  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AD 860002-85-3

RX(22) RCT AD 860002-85-3, AH 108-00-9  
PRO AN 854622-82-5  
SOL 64-17-5 EtOH  
CON reflux

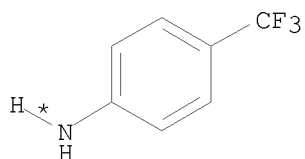
RX(31) RCT AN 854622-82-5, AU 112-13-0  
RGT AW 121-44-8 Et3N  
PRO BB 334801-64-8  
SOL 123-91-1 Dioxane

RX(130) OF 173 COMPOSED OF RX(7), RX(15), RX(23), RX(32)  
RX(130) C + Q + AH + AU ==> BC

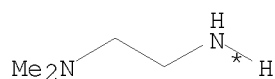
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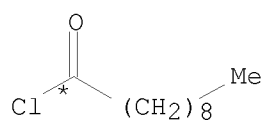
C



Q

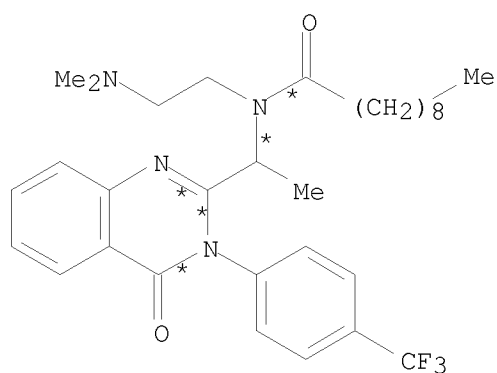


AH



AU

4  
STEPS  
→



BC

YIELD 55%

RX(7) RCT C 19165-26-5, Q 455-14-1  
RGT G 7719-12-2 PC13  
PRO R 860002-80-8  
SOL 108-88-3 PhMe

RX(15) RCT R 860002-80-8  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AE 860002-86-4

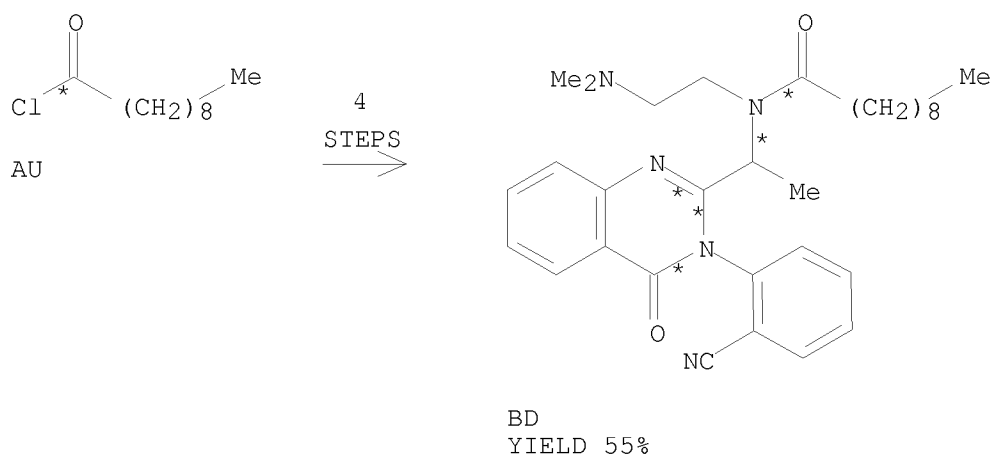
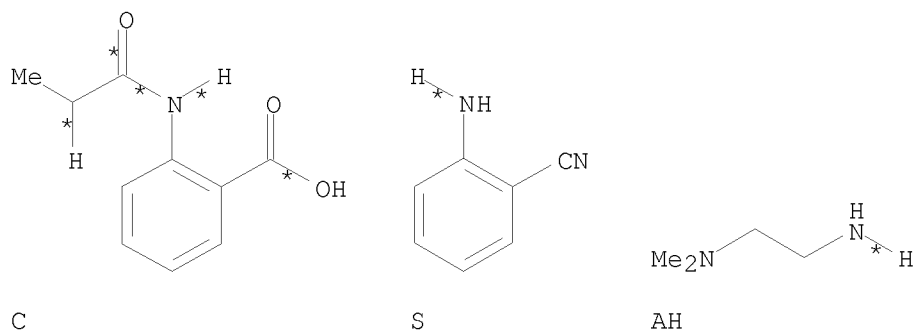
RX(23) RCT AE 860002-86-4, AH 108-00-9  
PRO AO 860002-91-1  
SOL 64-17-5 EtOH  
CON reflux

RX(32) RCT AO 860002-91-1, AU 112-13-0  
RGT AW 121-44-8 Et3N  
PRO BC 860002-96-6

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SOL 123-91-1 Dioxane

RX(132) OF 173 COMPOSED OF RX(8), RX(16), RX(24), RX(33)  
RX(132) C + S + AH + AU ==> BD



RX(8) RCT C 19165-26-5, S 1885-29-6  
RGT G 7719-12-2 PC13  
PRO T 860002-81-9  
SOL 108-88-3 PhMe

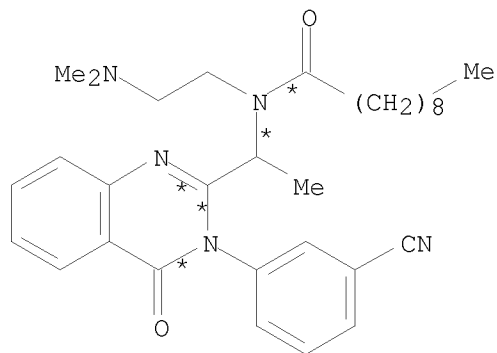
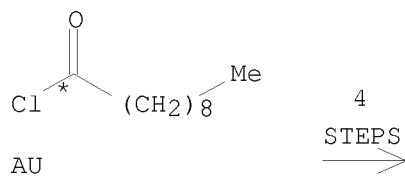
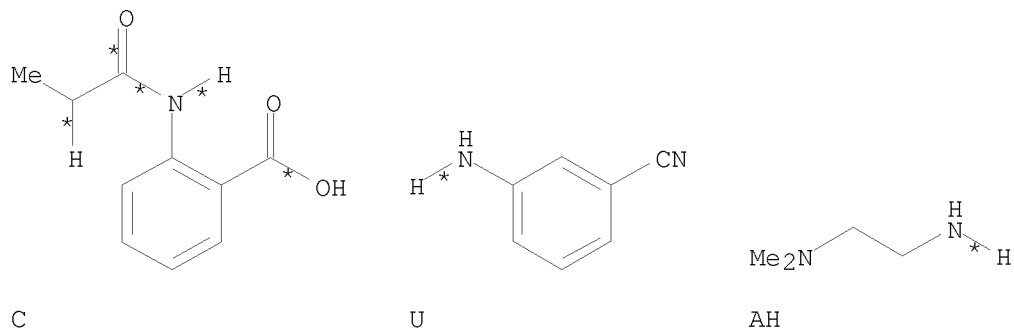
RX(16) RCT T 860002-81-9  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AF 860002-87-5

RX(24) RCT AF 860002-87-5, AH 108-00-9  
PRO AP 860002-92-2  
SOL 64-17-5 EtOH  
CON reflux

RX(33) RCT AP 860002-92-2, AU 112-13-0  
RGT AW 121-44-8 Et3N  
PRO BD 860002-97-7  
SOL 123-91-1 Dioxane

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RX(134) OF 173 COMPOSED OF RX(9), RX(17), RX(25), RX(34)  
RX(134) C + U + AH + AU ==> BE



BE  
YIELD 55%

RX(9) RCT C 19165-26-5, U 2237-30-1  
RGT G 7719-12-2 PC13  
PRO V 860002-82-0  
SOL 108-88-3 PhMe

RX(17) RCT V 860002-82-0  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AG 860002-88-6

RX(25) RCT AG 860002-88-6, AH 108-00-9  
PRO AQ 860002-93-3  
SOL 64-17-5 EtOH

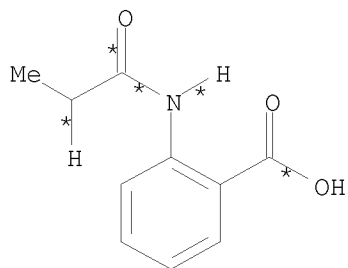


10/ 562,112

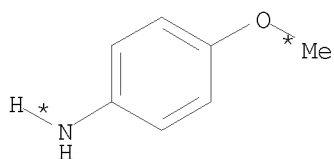
CON reflux

RX(34) RCT AQ 860002-93-3, AU 112-13-0  
RGT AW 121-44-8 Et3N  
PRO BE 860002-98-8  
SOL 123-91-1 Dioxane

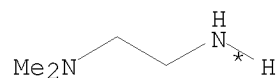
RX(155) OF 173 COMPOSED OF RX(3), RX(11), RX(19), RX(28), RX(35)  
RX(155) C + I + AH + AU + AL + BF ==> BG +  
BH



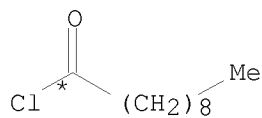
C



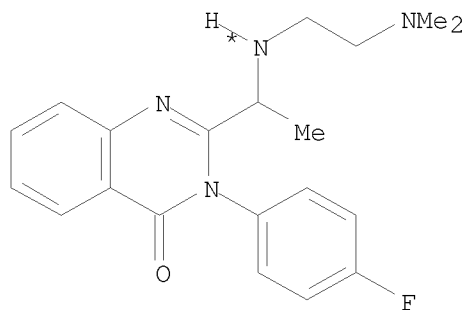
I



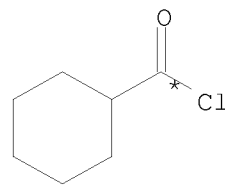
AH



AU



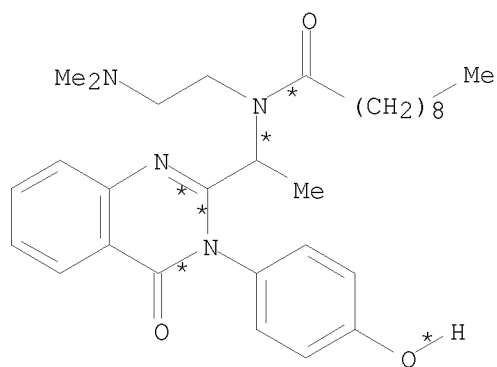
AL



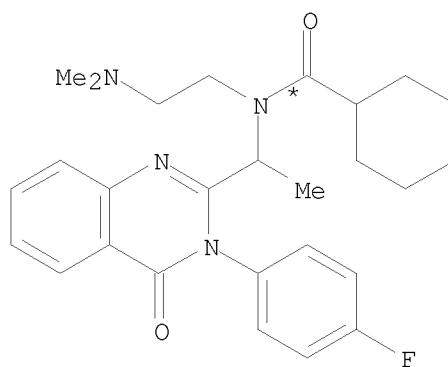
BF

5  
STEPS  
→

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BG  
YIELD 15%



BH  
YIELD 55%

```

RX(3)      RCT  C 19165-26-5, I 104-94-9
           RGT  G 7719-12-2 PC13
           PRO  J 50498-62-9
           SOL  108-88-3 PhMe

RX(11)     RCT  J 50498-62-9
           RGT  X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
           PRO  AA 473721-15-2

RX(19)     RCT  AA 473721-15-2, AH 108-00-9
           PRO  AK 473721-16-3
           SOL  64-17-5 EtOH
           CON  reflux

RX(28)     RCT  AK 473721-16-3, AU 112-13-0
           RGT  AW 121-44-8 Et3N
           PRO  AY 329190-30-9
           SOL  123-91-1 Dioxane

RX(35)     RCT  AL 329190-50-3, AY 329190-30-9, BF 2719-27-9
           RGT  AW 121-44-8 Et3N, AS 10294-33-4 BBr3
           PRO  BG 860002-99-9, BH 860003-00-5
           SOL  67-56-1 MeOH, 123-91-1 Dioxane

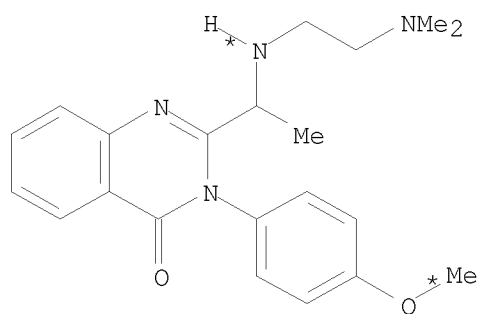
```

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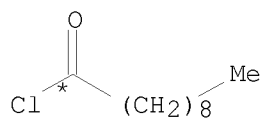
RX(157) OF 173 COMPOSED OF REACTION SEQUENCE RX(28), RX(35)
          AND REACTION SEQUENCE RX(4), RX(12), RX(20), RX(35)
...AK  +  AU  ==>  AY...
...  C  +  K  +  AH  +  AY  +  BF  ==>  BG  +  BH

```

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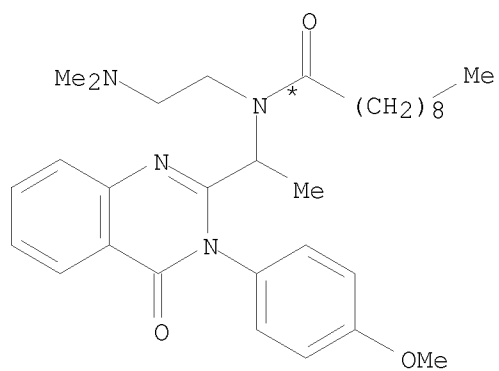


AK



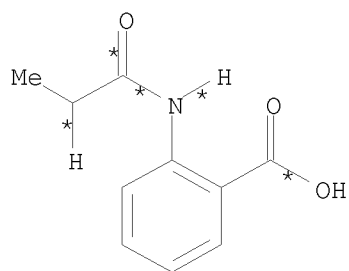
AU

4  
STEPS  
→

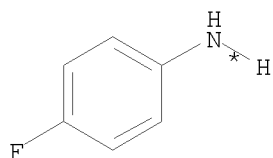


AY

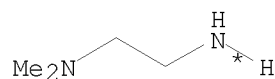
START NEXT REACTION SEQUENCE



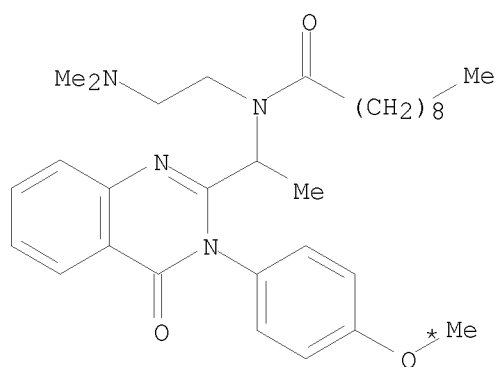
C



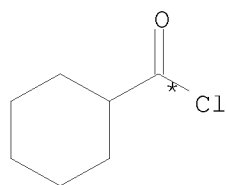
K



AH

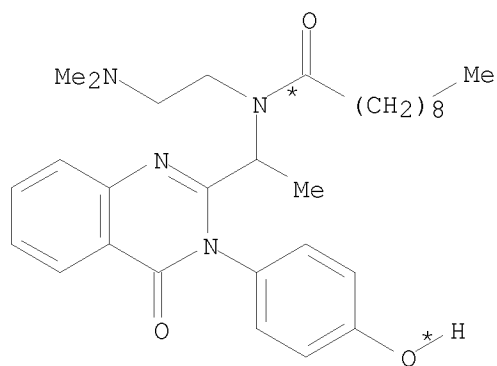


AY

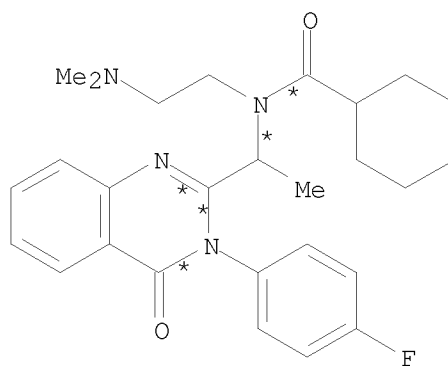


BF

4  
STEPS  
→



BG  
YIELD 15%



BH  
YIELD 55%

RX(28)	RCT	AK 473721-16-3, AU 112-13-0
	RGT	AW 121-44-8 Et3N
	PRO	AY 329190-30-9
	SOL	123-91-1 Dioxane
RX(4)	RCT	C 19165-26-5, K 371-40-4
	RGT	G 7719-12-2 PCl3
	PRO	L 329190-48-9
	SOL	108-88-3 PhMe
RX(12)	RCT	L 329190-48-9
	RGT	X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
	PRO	AB 329190-49-0
RX(20)	RCT	AB 329190-49-0, AH 108-00-9
	PRO	AL 329190-50-3
	SOL	64-17-5 EtOH
	CON	reflux
RX(35)	RCT	AL 329190-50-3, AY 329190-30-9, BF 2719-27-9
	RGT	AW 121-44-8 Et3N, AS 10294-33-4 BBr3

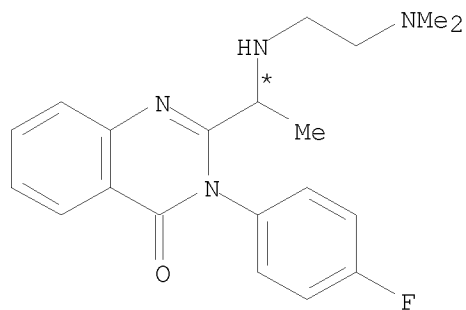
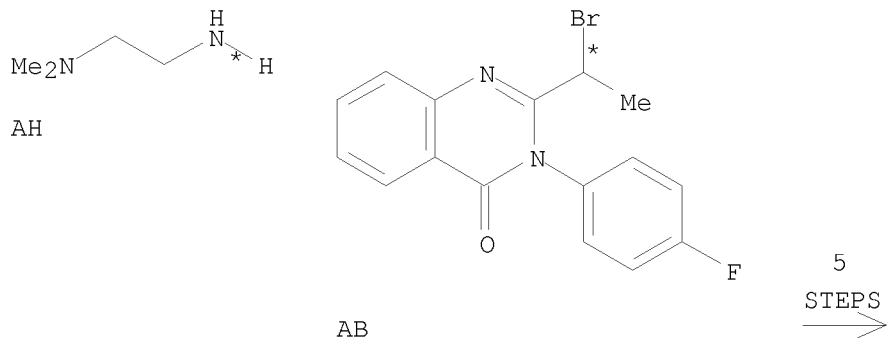
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PRO BG 860002-99-9, BH 860003-00-5  
SOL 67-56-1 MeOH, 123-91-1 Dioxane

RX(160) OF 173 COMPOSED OF REACTION SEQUENCE RX(20), RX(35)  
AND REACTION SEQUENCE RX(3), RX(11), RX(19), RX(28), RX(35)

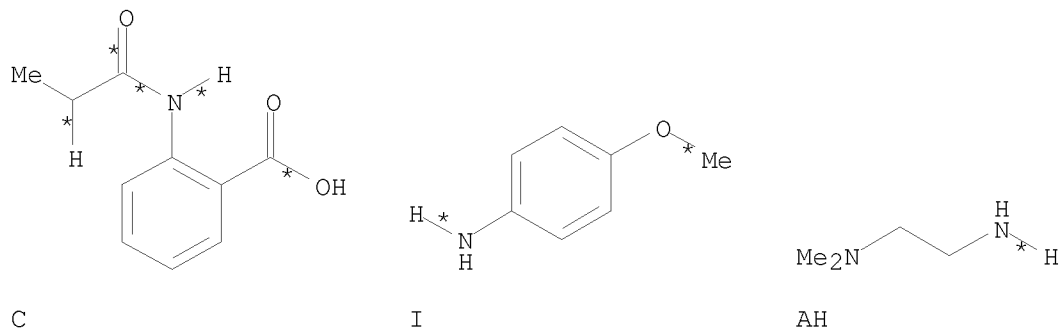
...AB + AH ==> AL...

... C + I + AH + AU + AL + BF ==> BG + BH

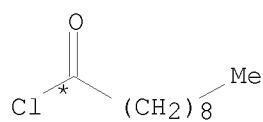


AL

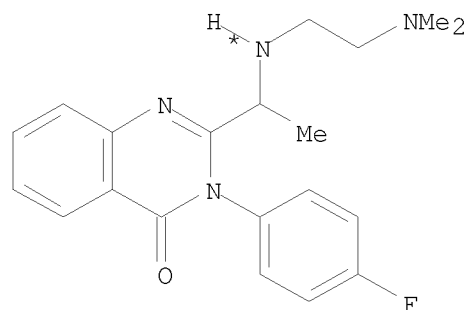
START NEXT REACTION SEQUENCE



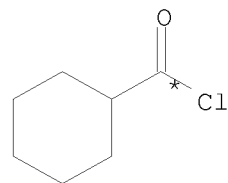
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AU

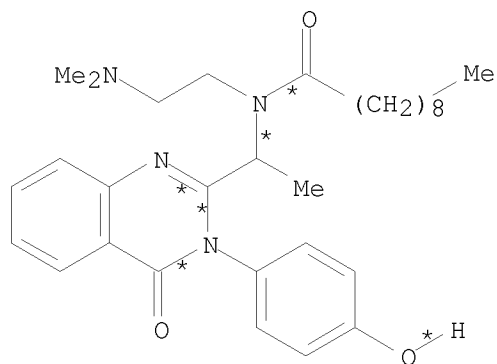


AL

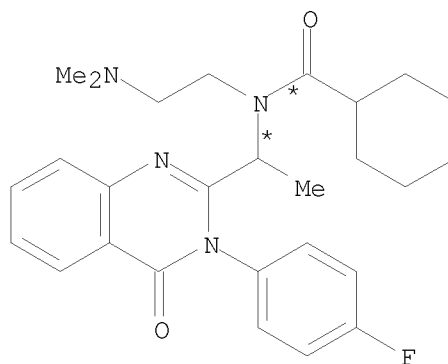


BF

5  
STEPS  
→



BG  
YIELD 15%



BH  
YIELD 55%

RX(20)	RCT	AB 329190-49-0, AH 108-00-9
	PRO	AL 329190-50-3
	SOL	64-17-5 EtOH
	CON	reflux
RX(3)	RCT	C 19165-26-5, I 104-94-9
	RGT	G 7719-12-2 PC13
	PRO	J 50498-62-9
	SOL	108-88-3 PhMe
RX(11)	RCT	J 50498-62-9
	RGT	X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
	PRO	AA 473721-15-2
RX(19)	RCT	AA 473721-15-2, AH 108-00-9
	PRO	AK 473721-16-3
	SOL	64-17-5 EtOH
	CON	reflux

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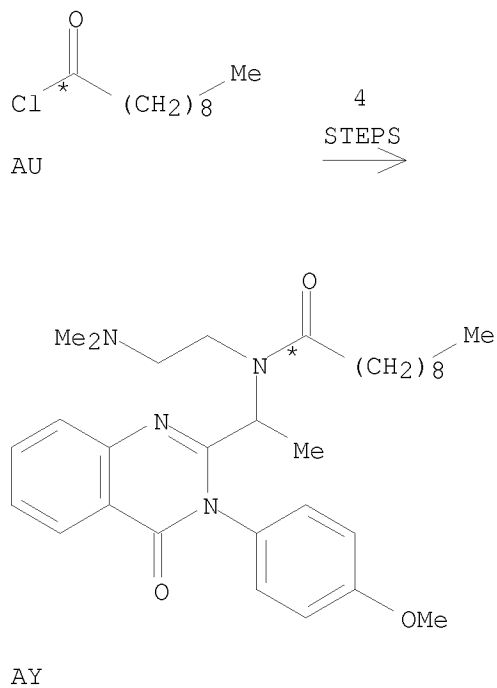
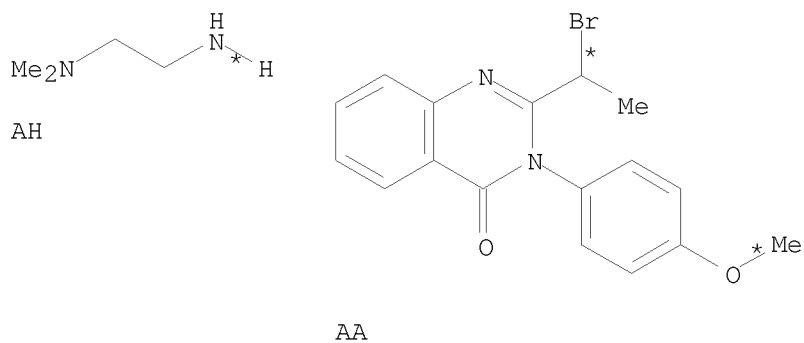
RX(28) RCT AK 473721-16-3, AU 112-13-0  
RGT AW 121-44-8 Et3N  
PRO AY 329190-30-9  
SOL 123-91-1 Dioxane

RX(35) RCT AL 329190-50-3, AY 329190-30-9, BF 2719-27-9  
RGT AW 121-44-8 Et3N, AS 10294-33-4 BBr3  
PRO BG 860002-99-9, BH 860003-00-5  
SOL 67-56-1 MeOH, 123-91-1 Dioxane

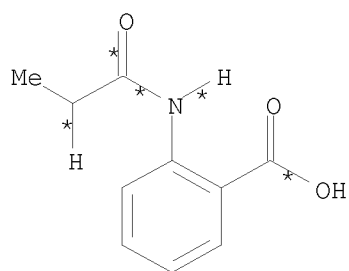
RX(163) OF 173 COMPOSED OF REACTION SEQUENCE RX(19), RX(28), RX(35)  
AND REACTION SEQUENCE RX(4), RX(12), RX(20), RX(35)

...AA + AH + AU ==> AY...

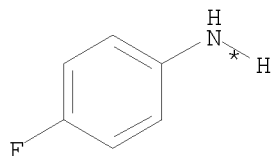
... C + K + AH + AY + BF ==> BG + BH



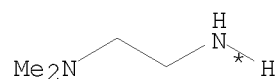
START NEXT REACTION SEQUENCE



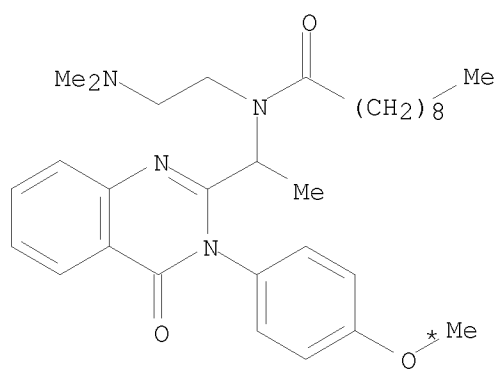
C



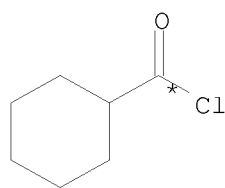
K



AH

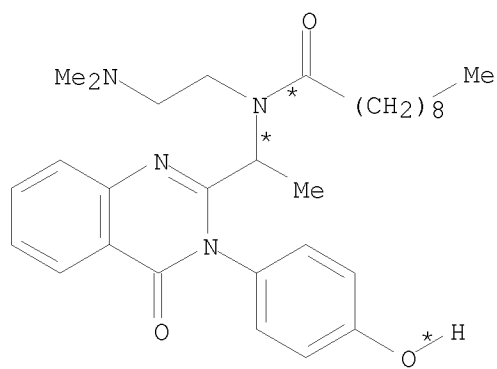


AY

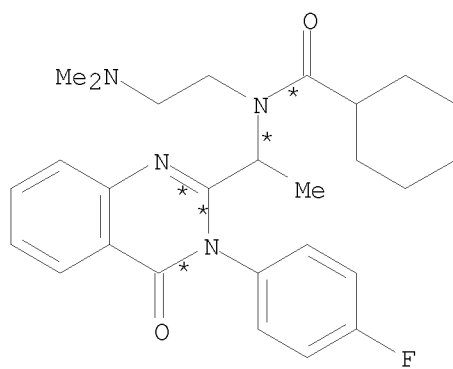


BF

4  
STEPS  
→



BG  
YIELD 15%



BH  
YIELD 55%

RX(19) RCT AA 473721-15-2, AH 108-00-9  
PRO AK 473721-16-3  
SOL 64-17-5 EtOH  
CON reflux

RX(28) RCT AK 473721-16-3, AU 112-13-0



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RGT AW 121-44-8 Et3N  
PRO AY 329190-30-9  
SOL 123-91-1 Dioxane

RX(4) RCT C 19165-26-5, K 371-40-4  
RGT G 7719-12-2 PC13  
PRO L 329190-48-9  
SOL 108-88-3 PhMe

RX(12) RCT L 329190-48-9  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AB 329190-49-0

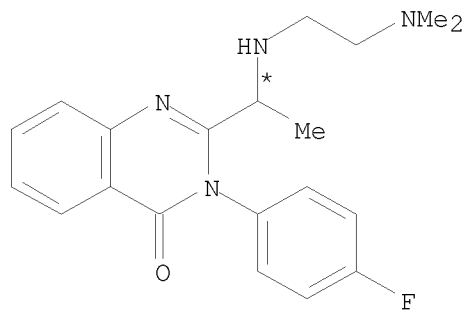
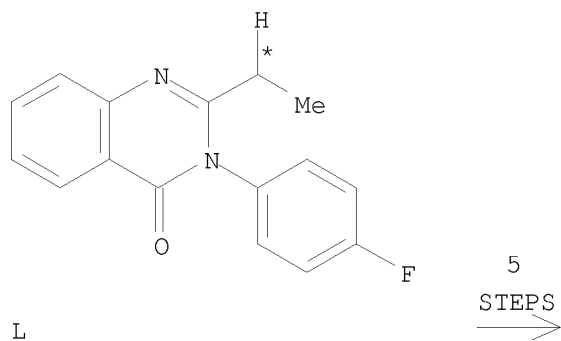
RX(20) RCT AB 329190-49-0, AH 108-00-9  
PRO AL 329190-50-3  
SOL 64-17-5 EtOH  
CON reflux

RX(35) RCT AL 329190-50-3, AY 329190-30-9, BF 2719-27-9  
RGT AW 121-44-8 Et3N, AS 10294-33-4 BBr3  
PRO BG 860002-99-9, BH 860003-00-5  
SOL 67-56-1 MeOH, 123-91-1 Dioxane

RX(166) OF 173 COMPOSED OF REACTION SEQUENCE RX(12), RX(20), RX(35)  
AND REACTION SEQUENCE RX(3), RX(11), RX(19), RX(28), RX(35)

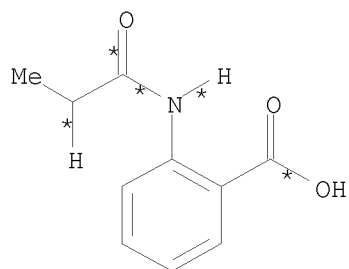
...L + AH ==> AL...

... C + I + AH + AU + AL + BF ==> BG + BH

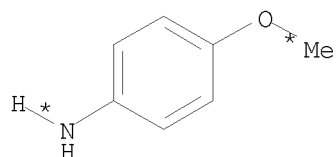


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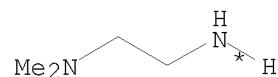
START NEXT REACTION SEQUENCE



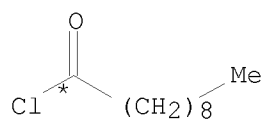
C



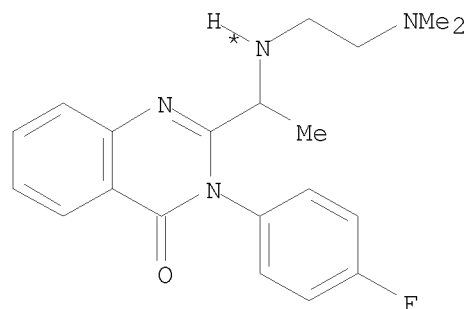
I



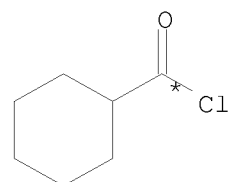
2 AH



AU

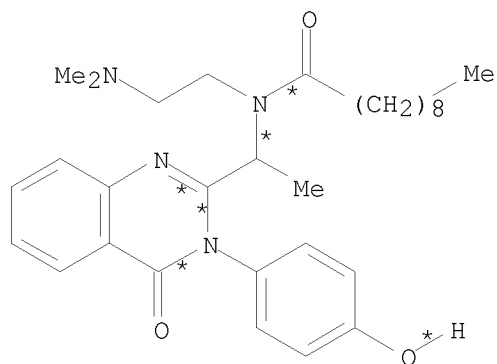


AL

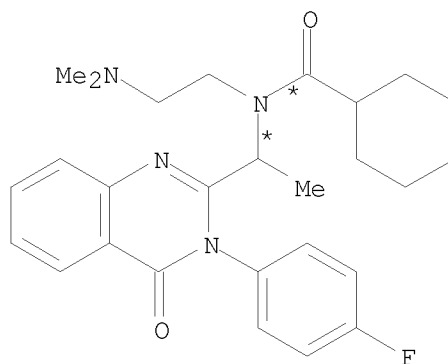


BF

5  
STEPS  
→



BG  
YIELD 15%



BH  
YIELD 55%

RX(12) RCT L 329190-48-9  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br<sub>2</sub>

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PRO AB 329190-49-0

RX(20) RCT AB 329190-49-0, AH 108-00-9  
PRO AL 329190-50-3  
SOL 64-17-5 EtOH  
CON reflux

RX(3) RCT C 19165-26-5, I 104-94-9  
RGT G 7719-12-2 PC13  
PRO J 50498-62-9  
SOL 108-88-3 PhMe

RX(11) RCT J 50498-62-9  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AA 473721-15-2

RX(19) RCT AA 473721-15-2, AH 108-00-9  
PRO AK 473721-16-3  
SOL 64-17-5 EtOH  
CON reflux

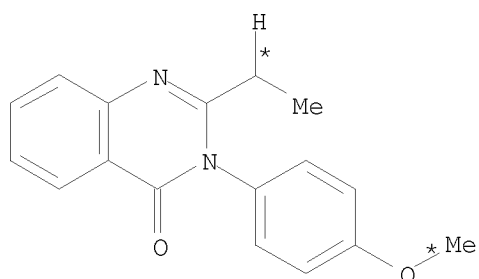
RX(28) RCT AK 473721-16-3, AU 112-13-0  
RGT AW 121-44-8 Et3N  
PRO AY 329190-30-9  
SOL 123-91-1 Dioxane

RX(35) RCT AL 329190-50-3, AY 329190-30-9, BF 2719-27-9  
RGT AW 121-44-8 Et3N, AS 10294-33-4 BBr3  
PRO BG 860002-99-9, BH 860003-00-5  
SOL 67-56-1 MeOH, 123-91-1 Dioxane

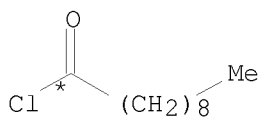
RX(168) OF 173 COMPOSED OF REACTION SEQUENCE RX(11), RX(19), RX(28), RX(35)  
AND REACTION SEQUENCE RX(4), RX(12), RX(20), RX(35)

...J + AH + AU ==> AY...

... C + K + AH + AY + BF ==> BG + BH

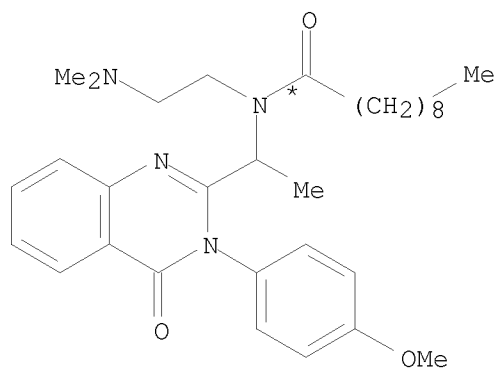


J



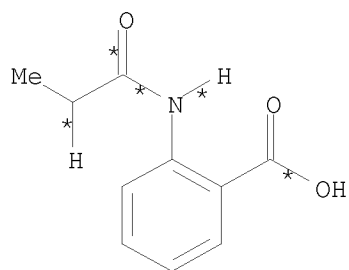
AU

4  
STEPS  
→

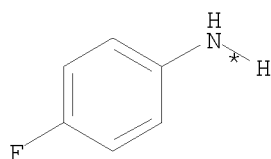


AY

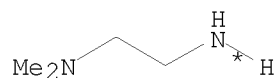
START NEXT REACTION SEQUENCE



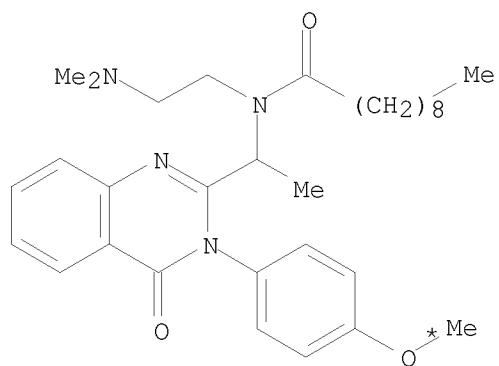
C



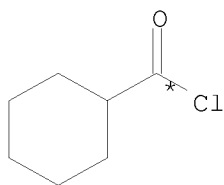
K



2 AH

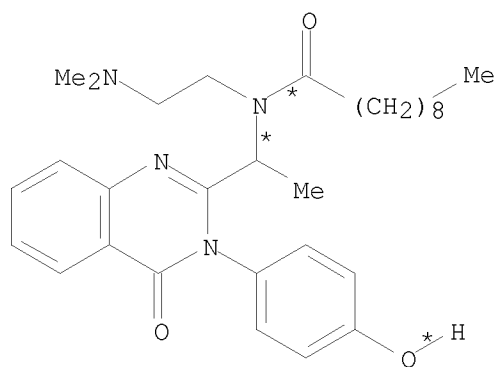


AY

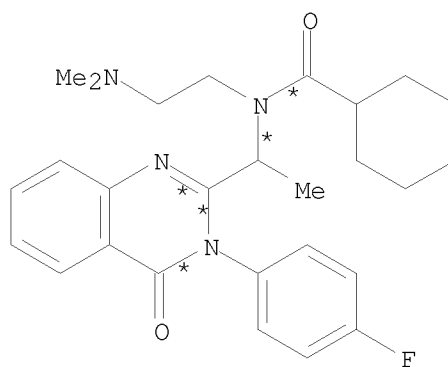


BF

4  
STEPS  
→



BG  
YIELD 15%



BH  
YIELD 55%

RX(11) RCT J 50498-62-9  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br<sub>2</sub>  
PRO AA 473721-15-2

RX(19) RCT AA 473721-15-2, AH 108-00-9  
PRO AK 473721-16-3  
SOL 64-17-5 EtOH  
CON reflux

RX(28) RCT AK 473721-16-3, AU 112-13-0  
RGT AW 121-44-8 Et<sub>3</sub>N  
PRO AY 329190-30-9  
SOL 123-91-1 Dioxane

RX(4) RCT C 19165-26-5, K 371-40-4  
RGT G 7719-12-2 PCl<sub>3</sub>  
PRO L 329190-48-9  
SOL 108-88-3 PhMe

RX(12) RCT L 329190-48-9  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br<sub>2</sub>  
PRO AB 329190-49-0

RX(20) RCT AB 329190-49-0, AH 108-00-9  
PRO AL 329190-50-3  
SOL 64-17-5 EtOH  
CON reflux

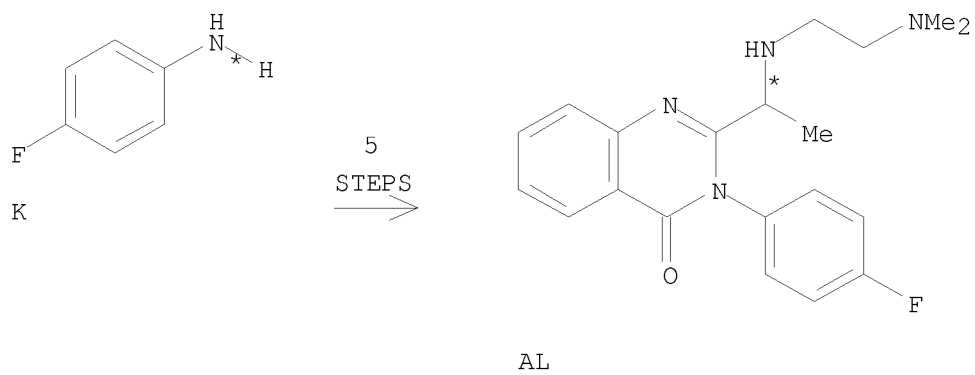
RX(35) RCT AL 329190-50-3, AY 329190-30-9, BF 2719-27-9  
RGT AW 121-44-8 Et<sub>3</sub>N, AS 10294-33-4 BBr<sub>3</sub>  
PRO BG 860002-99-9, BH 860003-00-5  
SOL 67-56-1 MeOH, 123-91-1 Dioxane

RX(170) OF 173 COMPOSED OF REACTION SEQUENCE RX(4), RX(12), RX(20), RX(35)  
AND REACTION SEQUENCE RX(3), RX(11), RX(19), RX(28), RX(35)

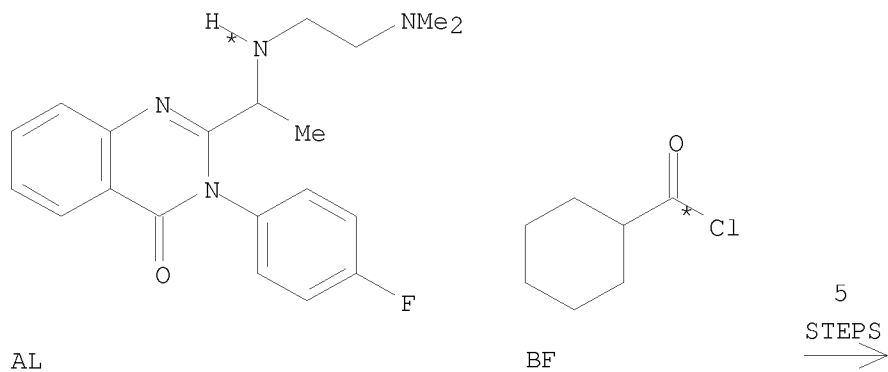
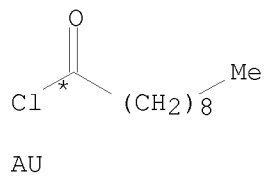
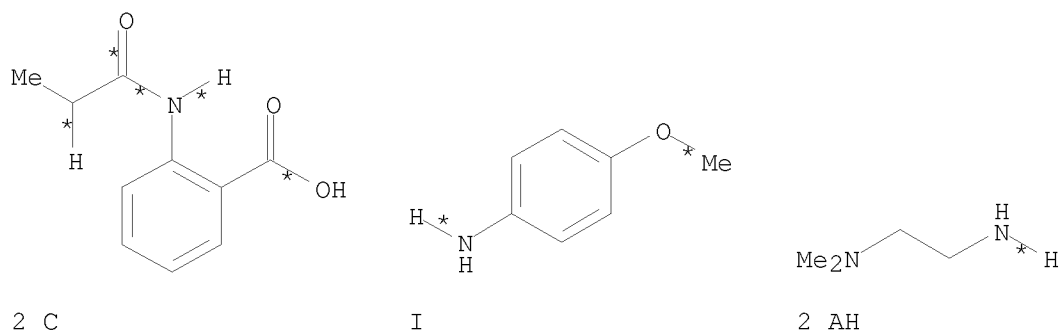
... C + K + AH ==> AL...

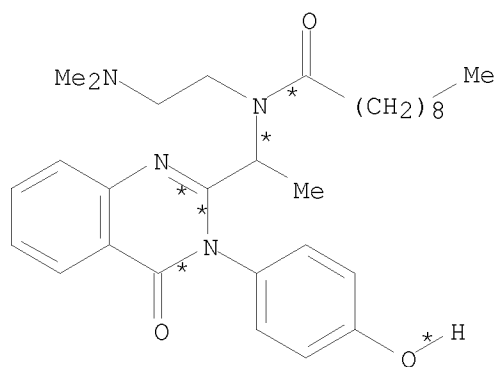
... C + I + AH + AU + AL + BF ==> BG + BH

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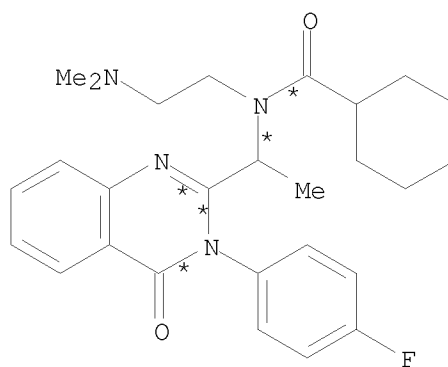


START NEXT REACTION SEQUENCE





BG  
YIELD 15%



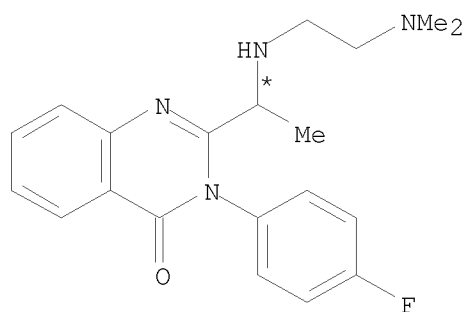
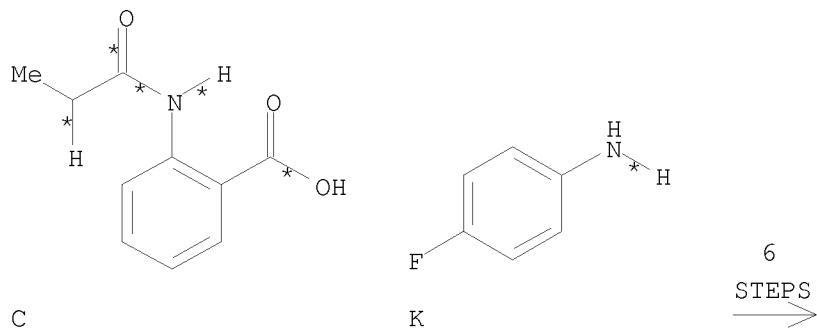
BH  
YIELD 55%

RX(4)	RCT	C 19165-26-5, K 371-40-4
	RGT	G 7719-12-2 PC13
	PRO	L 329190-48-9
	SOL	108-88-3 PhMe
RX(12)	RCT	L 329190-48-9
	RGT	X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
	PRO	AB 329190-49-0
RX(20)	RCT	AB 329190-49-0, AH 108-00-9
	PRO	AL 329190-50-3
	SOL	64-17-5 EtOH
	CON	reflux
RX(3)	RCT	C 19165-26-5, I 104-94-9
	RGT	G 7719-12-2 PC13
	PRO	J 50498-62-9
	SOL	108-88-3 PhMe
RX(11)	RCT	J 50498-62-9
	RGT	X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
	PRO	AA 473721-15-2
RX(19)	RCT	AA 473721-15-2, AH 108-00-9
	PRO	AK 473721-16-3
	SOL	64-17-5 EtOH
	CON	reflux
RX(28)	RCT	AK 473721-16-3, AU 112-13-0
	RGT	AW 121-44-8 Et3N
	PRO	AY 329190-30-9
	SOL	123-91-1 Dioxane
RX(35)	RCT	AL 329190-50-3, AY 329190-30-9, BF 2719-27-9
	RGT	AW 121-44-8 Et3N, AS 10294-33-4 BBr3
	PRO	BG 860002-99-9, BH 860003-00-5
	SOL	67-56-1 MeOH, 123-91-1 Dioxane

RX(171) OF 173 COMPOSED OF REACTION SEQUENCE RX(4), RX(12), RX(20), RX(35)

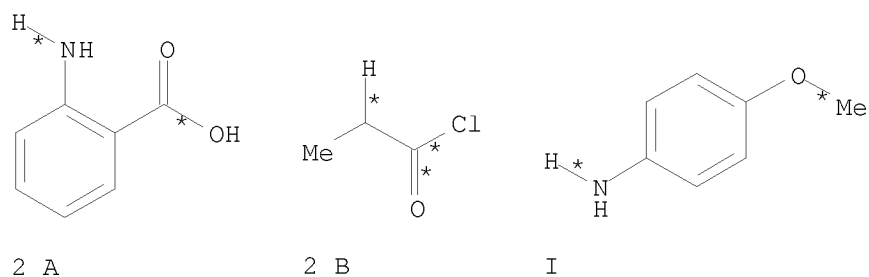
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AND REACTION SEQUENCE RX(1), RX(3), RX(11), RX(19), RX(28),  
 RX(35)  
 ... C + K + AH ==> AL...  
 ...2 A + 2 B + I + AH + AU + AL + BF ==> BG + BH



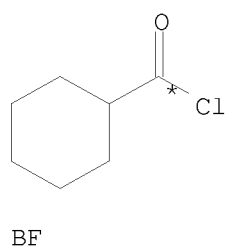
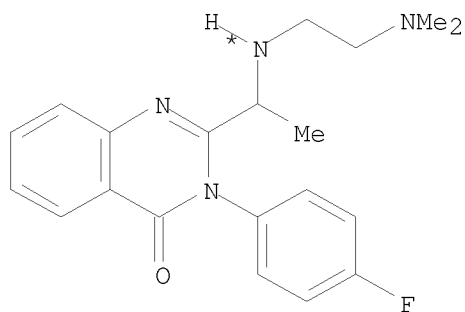
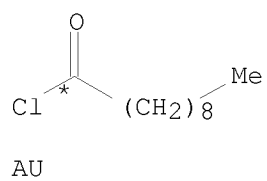
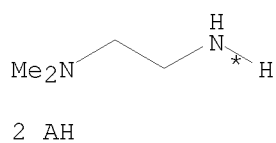
AL

START NEXT REACTION SEQUENCE

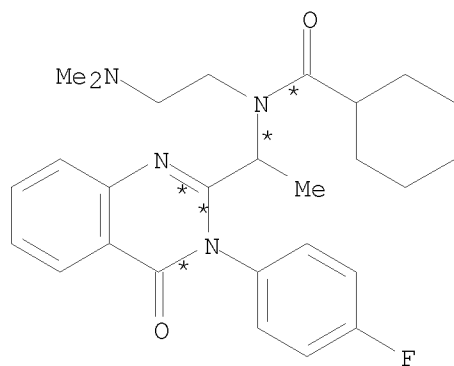
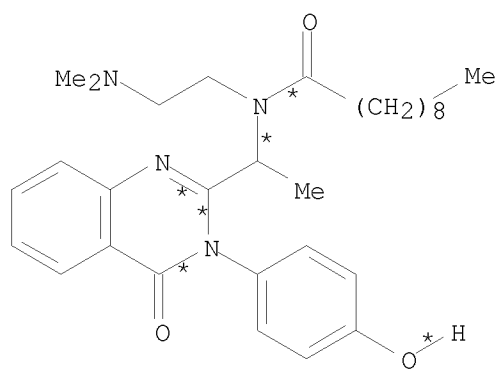




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6  
STEPS



RX(4)      RCT   C 19165-26-5, K 371-40-4  
              RGT   G 7719-12-2 PC13  
              PRO   L 329190-48-9

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SOL 108-88-3 PhMe

RX(12) RCT L 329190-48-9  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AB 329190-49-0

RX(20) RCT AB 329190-49-0, AH 108-00-9  
PRO AL 329190-50-3  
SOL 64-17-5 EtOH  
CON reflux

RX(1) RCT A 118-92-3, B 79-03-8  
PRO C 19165-26-5  
SOL 68-12-2 DMF

RX(3) RCT C 19165-26-5, I 104-94-9  
RGT G 7719-12-2 PCl3  
PRO J 50498-62-9  
SOL 108-88-3 PhMe

RX(11) RCT J 50498-62-9  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AA 473721-15-2

RX(19) RCT AA 473721-15-2, AH 108-00-9  
PRO AK 473721-16-3  
SOL 64-17-5 EtOH  
CON reflux

RX(28) RCT AK 473721-16-3, AU 112-13-0  
RGT AW 121-44-8 Et3N  
PRO AY 329190-30-9  
SOL 123-91-1 Dioxane

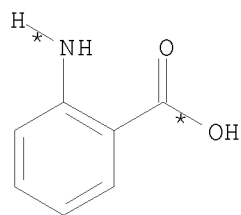
RX(35) RCT AL 329190-50-3, AY 329190-30-9, BF 2719-27-9  
RGT AW 121-44-8 Et3N, AS 10294-33-4 BBr3  
PRO BG 860002-99-9, BH 860003-00-5  
SOL 67-56-1 MeOH, 123-91-1 Dioxane

RX(172) OF 173 COMPOSED OF REACTION SEQUENCE RX(1), RX(4), RX(12), RX(20),  
RX(35)

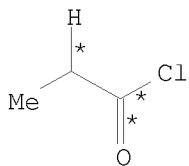
AND REACTION SEQUENCE RX(3), RX(11), RX(19), RX(28), RX(35)

...A + B + K + AH ==> AL...

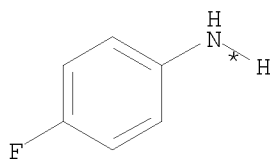
... C + I + AH + AU + AL + BF ==> BG + BH



A



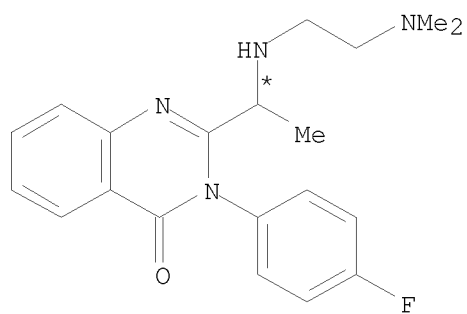
B



K

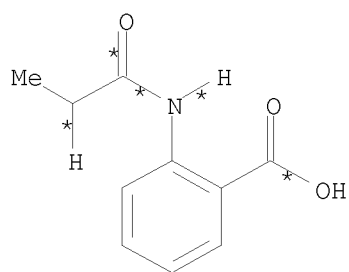
5  
STEPS  
→

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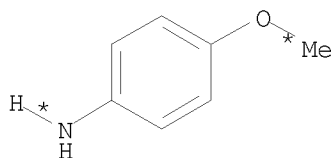


AL

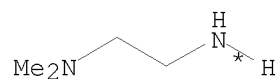
START NEXT REACTION SEQUENCE



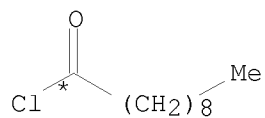
C



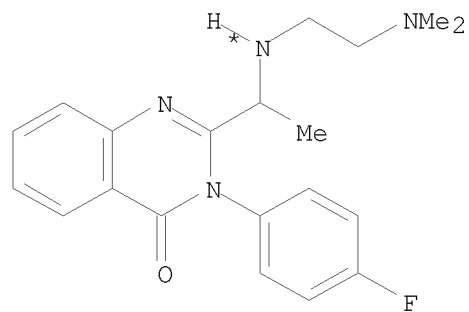
I



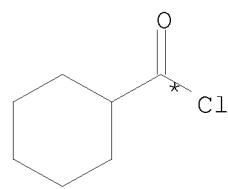
2 AH



AU

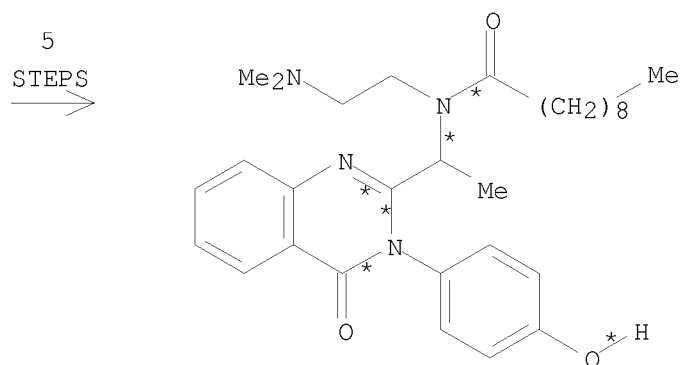


AL

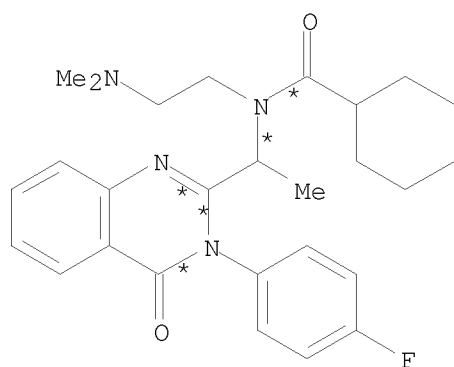


BF

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BG  
YIELD 15%



BH  
YIELD 55%

RX(1)	RCT	A 118-92-3, B 79-03-8
	PRO	C 19165-26-5
	SOL	68-12-2 DMF
RX(4)	RCT	C 19165-26-5, K 371-40-4
	RGT	G 7719-12-2 PC13
	PRO	L 329190-48-9
	SOL	108-88-3 PhMe
RX(12)	RCT	L 329190-48-9
	RGT	X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
	PRO	AB 329190-49-0
RX(20)	RCT	AB 329190-49-0, AH 108-00-9
	PRO	AL 329190-50-3
	SOL	64-17-5 EtOH
	CON	reflux
RX(3)	RCT	C 19165-26-5, I 104-94-9
	RGT	G 7719-12-2 PC13

PRO J 50498-62-9  
SOL 108-88-3 PhMe

RX(11) RCT J 50498-62-9  
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2  
PRO AA 473721-15-2

RX(19) RCT AA 473721-15-2, AH 108-00-9  
PRO AK 473721-16-3  
SOL 64-17-5 EtOH  
CON reflux

RX(28) RCT AK 473721-16-3, AU 112-13-0  
RGT AW 121-44-8 Et3N  
PRO AY 329190-30-9  
SOL 123-91-1 Dioxane

RX(35) RCT AL 329190-50-3, AY 329190-30-9, BF 2719-27-9  
RGT AW 121-44-8 Et3N, AS 10294-33-4 BBr3  
PRO BG 860002-99-9, BH 860003-00-5  
SOL 67-56-1 MeOH, 123-91-1 Dioxane

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 50 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 143:26556 CASREACT

TITLE: Synthetic studies on 3-arylquinazolin-4-ones:  
intramolecular nucleophilic aromatic substitution  
reaction of 2-carboxamido-3-arylquinazolin-4-ones and  
its application to the synthesis of secondary aryl  
amines

AUTHOR(S): Fuwa, Haruhiko; Kobayashi, Toshitake; Tokitoh,  
Takashi; Torii, Yukiko; Natsugari, Hideaki

CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, University  
of Tokyo, Bunkyo-ku, Tokyo, 113-0033, Japan

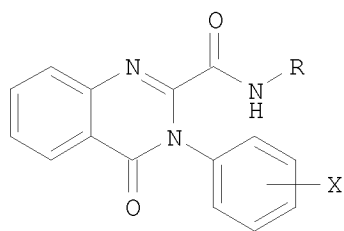
SOURCE: Tetrahedron (2005), 61(17), 4297-4312  
CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier B.V.

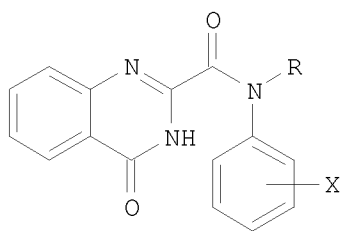
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



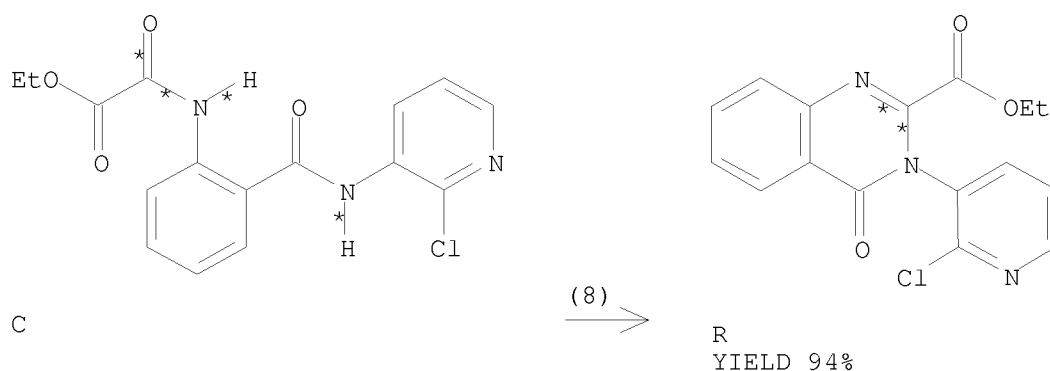
I



II

AB 2-Carboxamido-3-arylquinazolin-4-ones were prepared via acylation of aromatic amines, cyclodehydration, transesterification, and amidation. A novel intramol. nucleophilic aromatic substitution (SNAr) reaction of 2-carboxamido-3-arylquinazolin-4-ones, a potentially useful scaffold in the field of medicinal chemical, is described. E.g., treatment of 2-carboxamido-3-arylquinazolin-4-ones I (X = 4-CF<sub>3</sub>, o-CO<sub>2</sub>Me, 4-CN, etc.; R = CH<sub>2</sub>Ph, Ph, Bu) with NaH in DMF gave migrated products II. The synthetic utility of the SNAr reaction as a tool for the synthesis of secondary aryl amines, including diaryl amines, is also demonstrated. Thus, reaction of the 2-ethoxycarbonyl-3-arylquinazolin-4-ones and primary amines in the presence of a base induced a cascade process comprised of amide formation, intramol. SNAr reaction, and cleavage of the resultant tertiary amide to yield (in one-pot) secondary aryl amines.

RX(8) OF 229 ...C ==> R...



RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)<sub>2</sub>, T 7553-56-2 I<sub>2</sub>, U 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

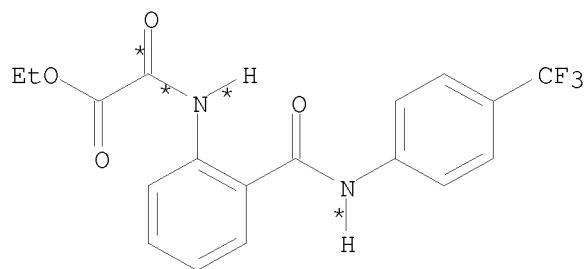
RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO R 830324-68-0

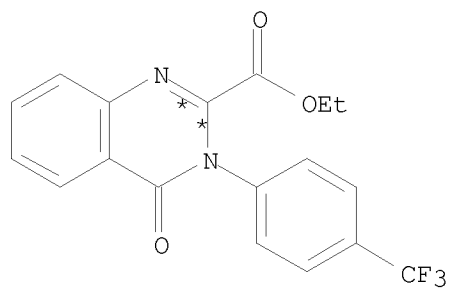
RX(9) OF 229 ...G ==> X...

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G

(9)  $\longrightarrow$



X

YIELD 82%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

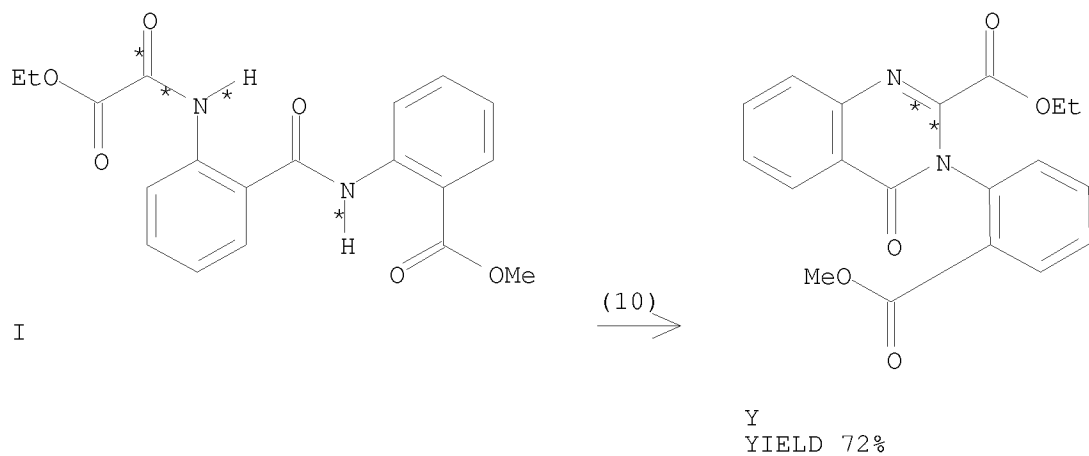
RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO X 361180-29-2

RX(10) OF 229 ...I ==> Y...

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RX(10) RCT I 852534-80-6

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

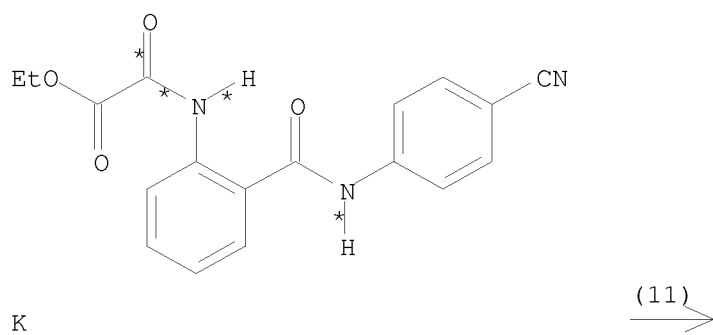
STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

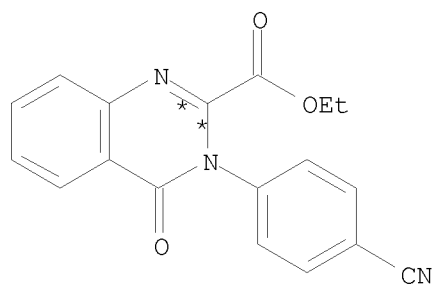
PRO Y 852534-83-9

RX(11) OF 229 ...K ==> Z...





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Z  
YIELD 60%

RX(11) RCT K 852534-81-7

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

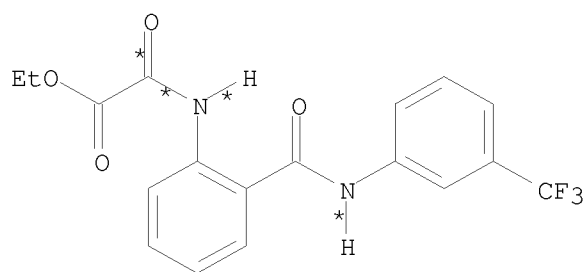
STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO Z 830325-00-3

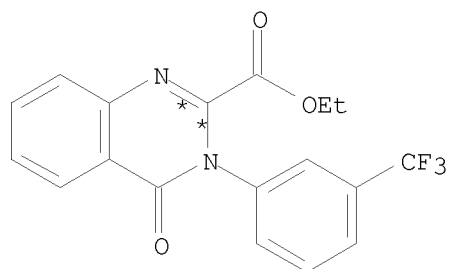
RX(12) OF 229 ...M ==> AA...



M

(12)

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AA  
YIELD 77%

RX(12) RCT M 852534-82-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)<sub>2</sub>, T 7553-56-2 I<sub>2</sub>, U 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

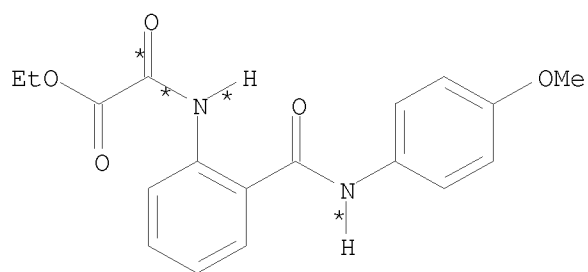
STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO AA 310423-02-0

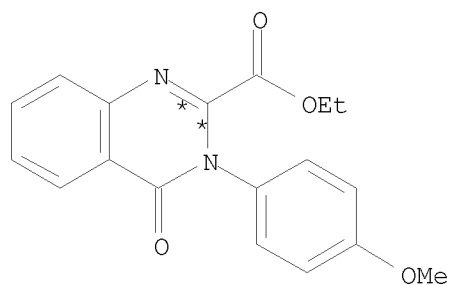
RX(13) OF 229 ...O ==> AB...



O

(13)  $\longrightarrow$

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AB  
YIELD 46%

RX(13) RCT O 30838-15-4

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

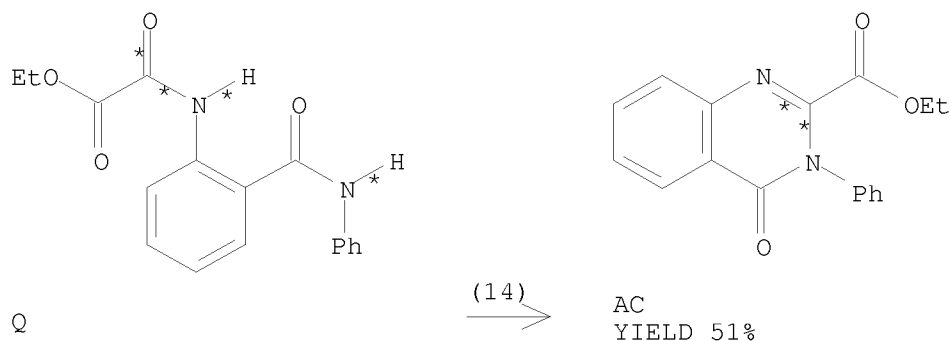
STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO AB 30838-19-8

RX(14) OF 229 ...Q ==> AC...



RX(14) RCT Q 30838-11-0

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

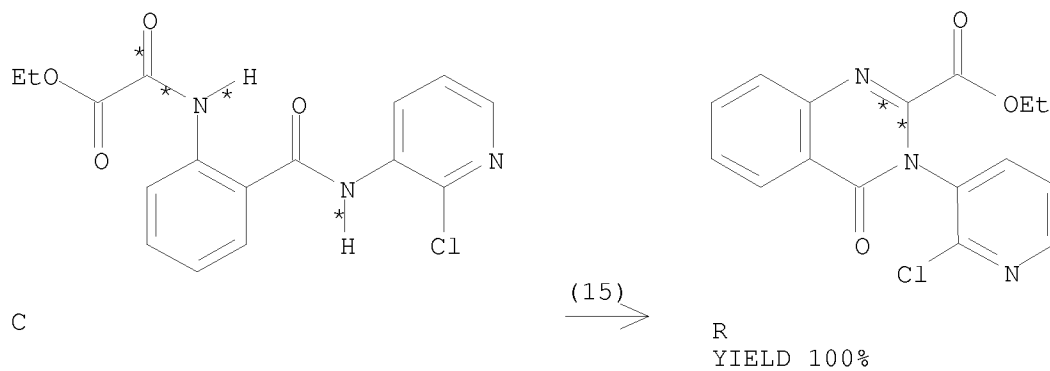
RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

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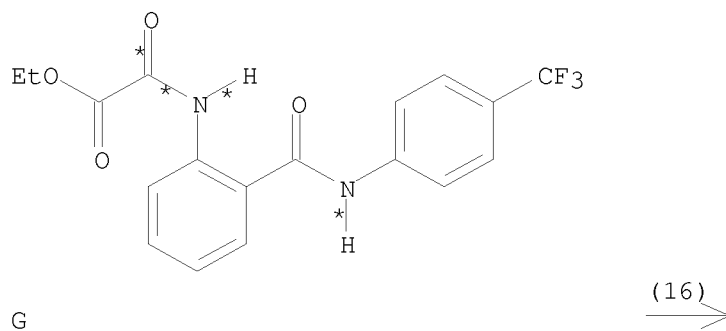
PRO AC 30838-16-5

RX(15) OF 229 C ==> R

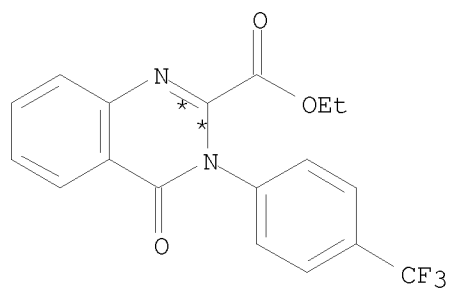


RX(15) RCT C 830324-66-8  
RGT AD 121-44-8 Et3N, AE 75-77-4 Me3SiCl  
PRO R 830324-68-0  
SOL 107-06-2 ClCH2CH2Cl  
CON 1.5 hours, reflux

RX(16) OF 229 G ==> X



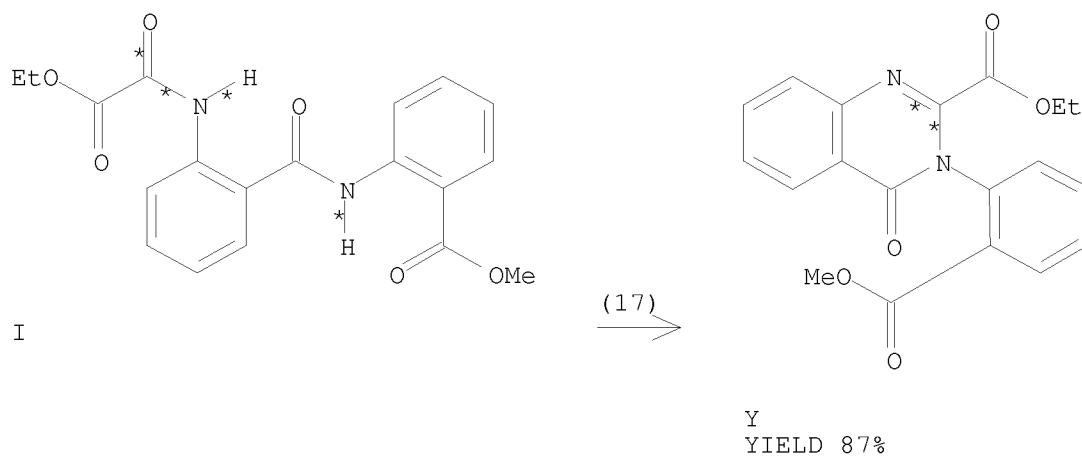
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X  
YIELD 94%

RX(16) RCT G 852534-79-3  
RGT AD 121-44-8 Et3N, AE 75-77-4 Me3SiCl  
PRO X 361180-29-2  
SOL 107-06-2 ClCH2CH2Cl  
CON 1.5 hours, reflux

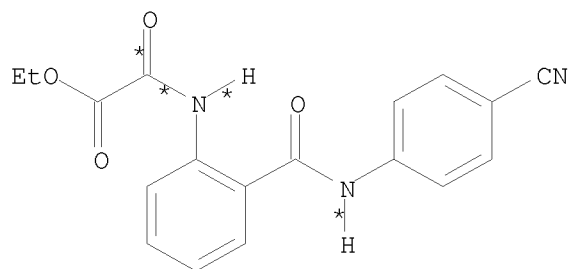
RX(17) OF 229 I ==> Y



RX(17) RCT I 852534-80-6  
RGT AD 121-44-8 Et3N, AE 75-77-4 Me3SiCl  
PRO Y 852534-83-9  
SOL 107-06-2 ClCH2CH2Cl  
CON 1.5 hours, reflux

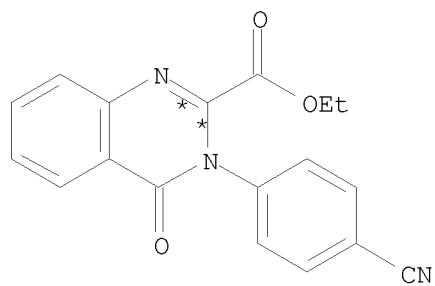
RX(18) OF 229 K ==> Z

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K

(18)  $\longrightarrow$

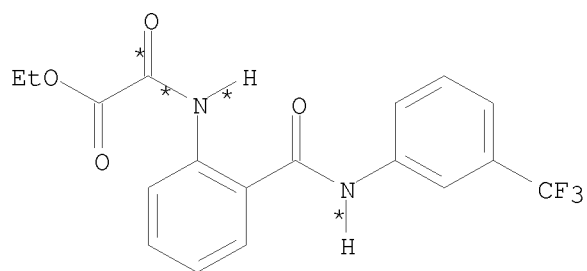


Z

YIELD 89%

RX(18)     RCT   K 852534-81-7  
             RGT   AD 121-44-8 Et3N, AE 75-77-4 Me3SiCl  
             PRO   Z 830325-00-3  
             SOL   107-06-2 ClCH2CH2Cl  
             CON   1.5 hours, reflux

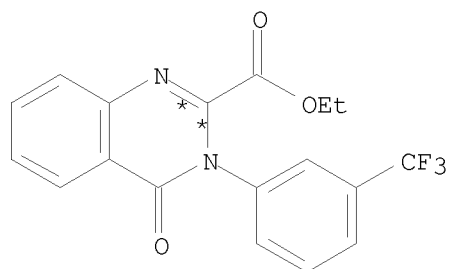
RX(19) OF 229     M    ==>   AA



M

(19)  $\longrightarrow$

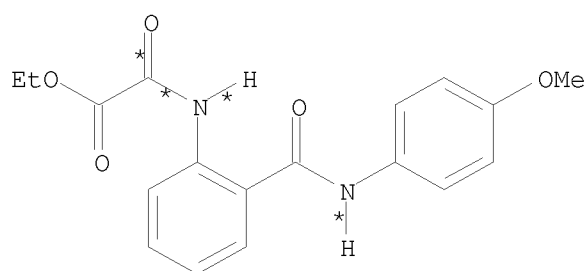
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AA  
YIELD 98%

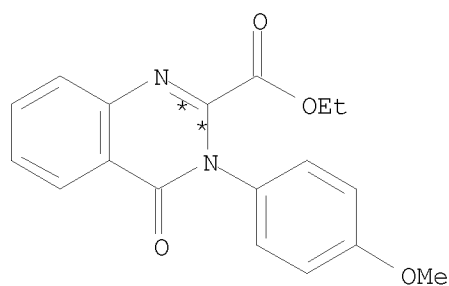
RX(19)      RCT    M 852534-82-8  
              RGT    AD 121-44-8 Et3N, AE 75-77-4 Me3SiCl  
              PRO    AA 310423-02-0  
              SOL    107-06-2 ClCH2CH2Cl  
              CON    1.5 hours, reflux

RX(20) OF 229      O    ==>    AB



O

(20)



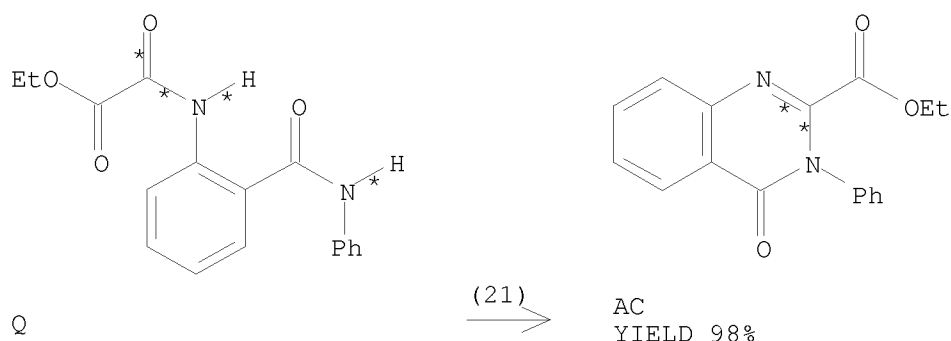
AB  
YIELD 84%

RX(20)      RCT    O 30838-15-4

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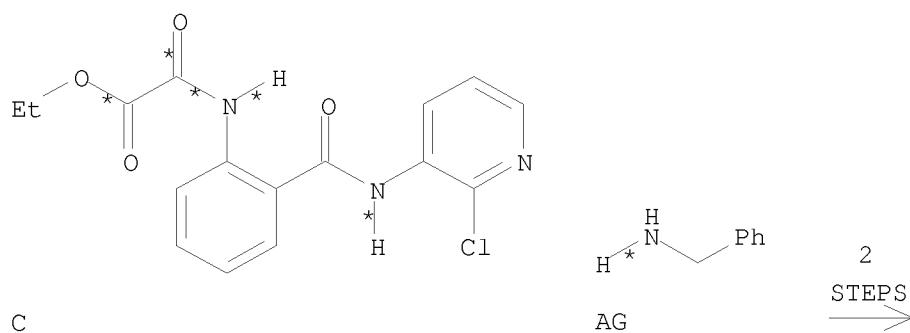
RGT AD 121-44-8 Et3N, AE 75-77-4 Me3SiCl  
PRO AB 30838-19-8  
SOL 107-06-2 ClCH2CH2Cl  
CON 1.5 hours, reflux

RX(21) OF 229 Q ==> AC



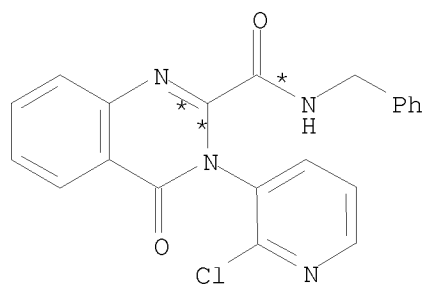
RX(21) RCT Q 30838-11-0  
RGT AD 121-44-8 Et3N, AE 75-77-4 Me3SiCl  
PRO AC 30838-16-5  
SOL 107-06-2 ClCH2CH2Cl  
CON 1.5 hours, reflux

RX(80) OF 229 COMPOSED OF RX(8), RX(22)  
RX(80) C + AG ==> AH





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AH  
YIELD 100%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO R 830324-68-0

RX(22) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 1 hour, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0

CON 7 hours, room temperature

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

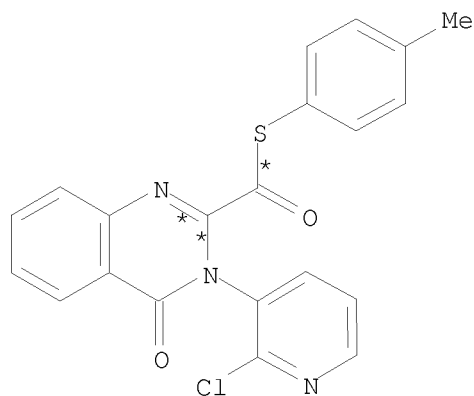
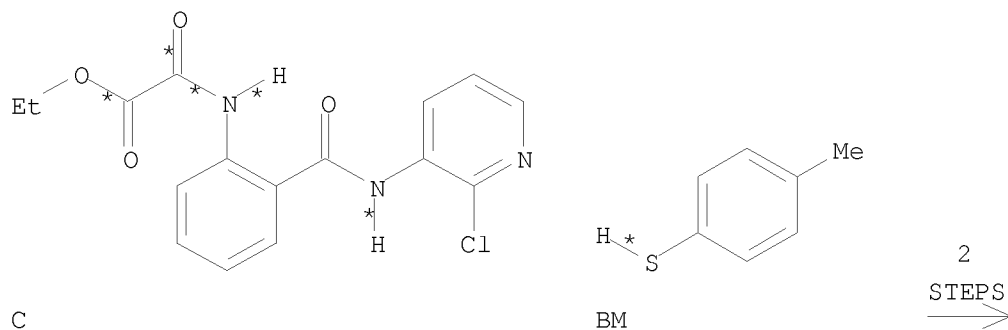
CON 0 deg C

PRO AH 830324-76-0

RX(81) OF 229 COMPOSED OF RX(8), RX(38)

RX(81) C + BM ==> AR

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AR  
YIELD 87%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)<sub>2</sub>, T 7553-56-2 I<sub>2</sub>, U 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

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STAGE(2)

RCT R 830324-68-0

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

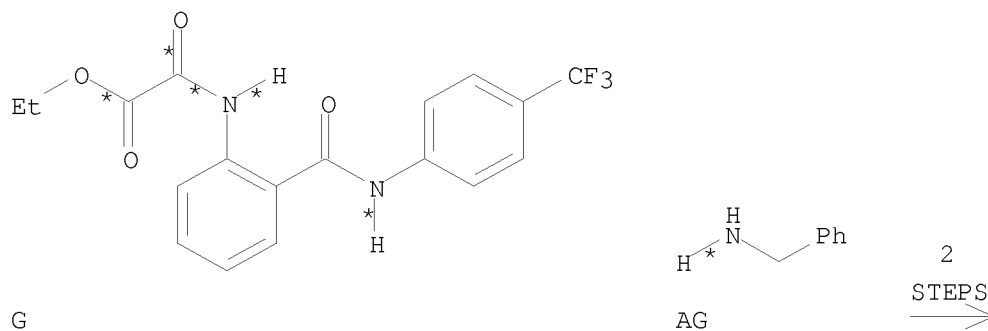
SOL 7732-18-5 Water

CON 0 deg C

PRO AR 830324-69-1

RX(88) OF 229 COMPOSED OF RX(9), RX(23)

RX(88) G + AG ==> AM



AM  
YIELD 76%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)<sub>2</sub>, T 7553-56-2 I<sub>2</sub>, U 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

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PRO X 361180-29-2

RX(23) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 1 hour, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT X 361180-29-2

CON 7 hours, room temperature

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

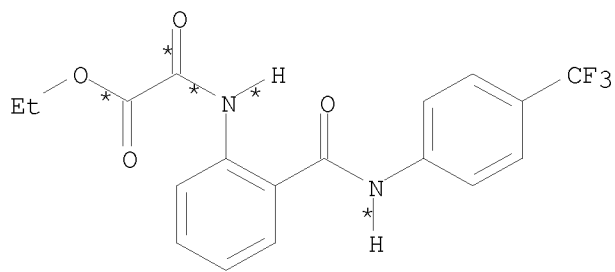
SOL 7732-18-5 Water

CON 0 deg C

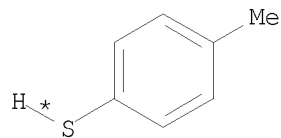
PRO AM 830324-84-0

RX(89) OF 229 COMPOSED OF RX(9), RX(39)

RX(89) G + BM ==> AZ



G



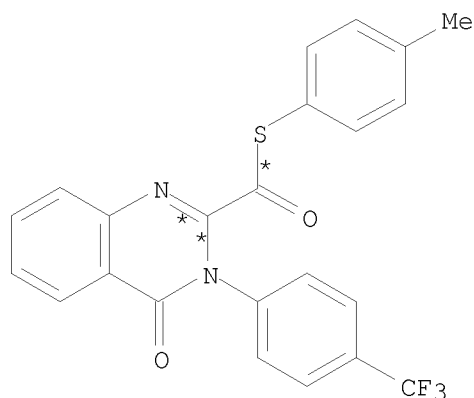
BM

2

STEPS



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AZ  
YIELD 60%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO X 361180-29-2

RX(39) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT X 361180-29-2

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

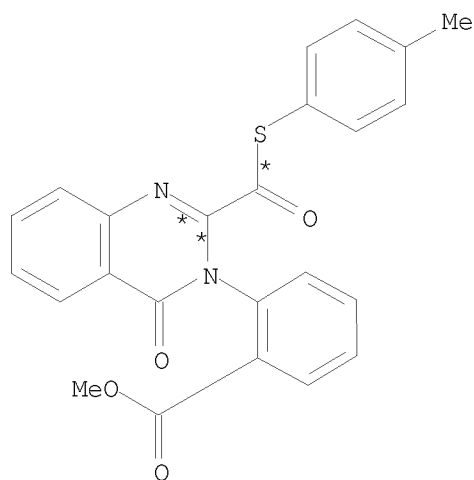
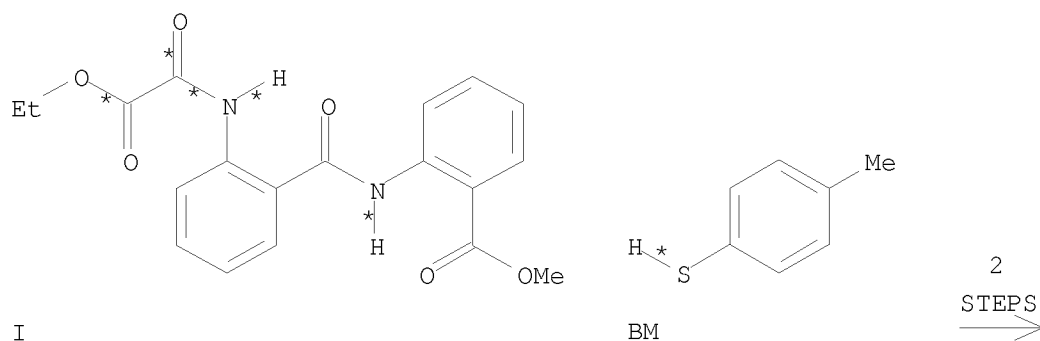
CON 0 deg C

PRO AZ 852534-84-0

RX(92) OF 229 COMPOSED OF RX(10), RX(40)

RX(92) I + BM ==> AV

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AV  
YIELD 91%

RX(10) RCT I 852534-80-6

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO Y 852534-83-9

RX(40) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

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SUBSTAGE(2) 30 minutes, room temperature  
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT Y 852534-83-9

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

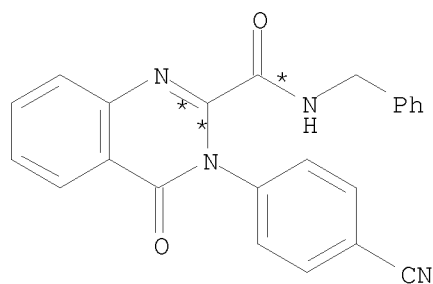
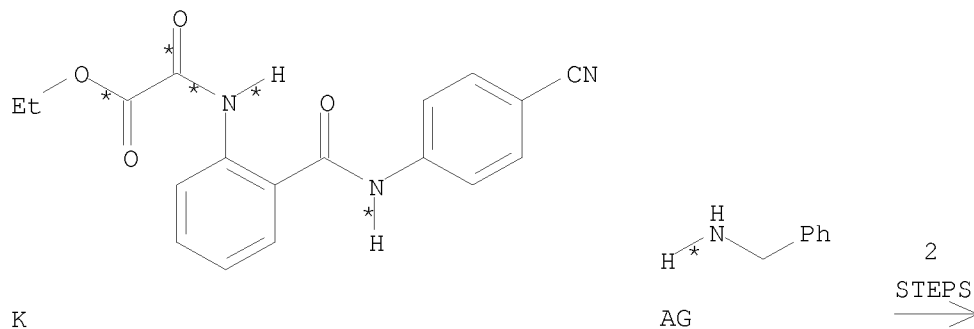
SOL 7732-18-5 Water

CON 0 deg C

PRO AV 852534-85-1

RX(93) OF 229 COMPOSED OF RX(11), RX(24)

RX(93) K + AG ==> AN



AN  
YIELD 53%

RX(11) RCT K 852534-81-7

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

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RGT V 123-75-1 Pyrrolidine  
SOL 109-99-9 THF

PRO Z 830325-00-3

RX(24) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe<sub>3</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 110-54-3 Hexane  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 1 hour, room temperature  
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT Z 830325-00-3  
CON 7 hours, room temperature

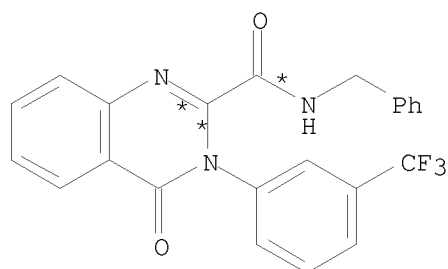
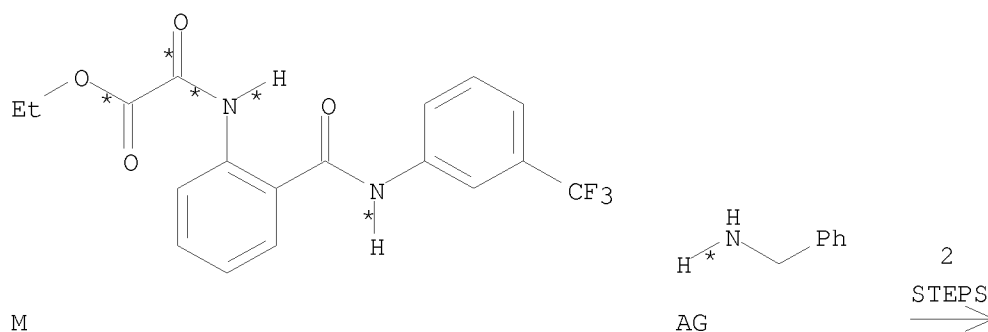
STAGE(3)

RGT AJ 304-59-6 Rochelle salt  
SOL 7732-18-5 Water  
CON 0 deg C

PRO AN 830324-86-2

RX(96) OF 229 COMPOSED OF RX(12), RX(25)

RX(96) M + AG ==> AO



AO  
YIELD 93%



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RX(12) RCT M 852534-82-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO AA 310423-02-0

RX(25) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 1 hour, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT AA 310423-02-0

CON 7 hours, room temperature

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

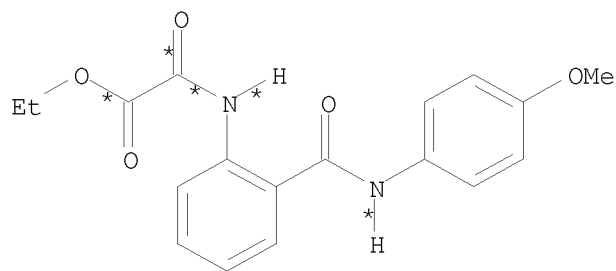
SOL 7732-18-5 Water

CON 0 deg C

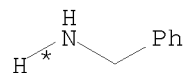
PRO AO 852534-86-2

RX(97) OF 229 COMPOSED OF RX(13), RX(26)

RX(97) O + AG ==> AP



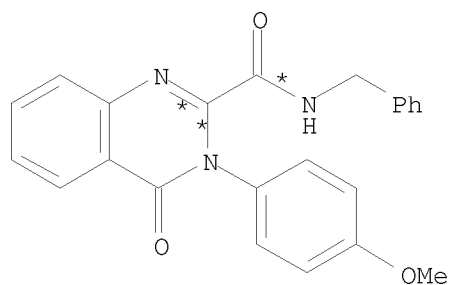
O



AG

2  
STEPS  
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AP  
YIELD 96%

RX(13) RCT O 30838-15-4

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO AB 30838-19-8

RX(26) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 1 hour, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT AB 30838-19-8

CON 7 hours, room temperature

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

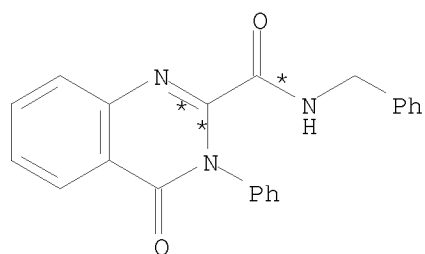
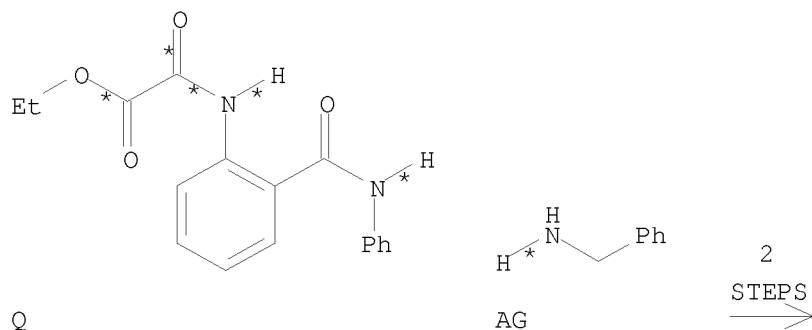
CON 0 deg C

PRO AP 852534-87-3

RX(98) OF 229 COMPOSED OF RX(14), RX(27)

RX(98) Q + AG ==> AQ

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AQ  
YIELD 78%

RX(14) RCT Q 30838-11-0

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO AC 30838-16-5

RX(27) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 1 hour, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT AC 30838-16-5

CON 7 hours, room temperature

STAGE(3)

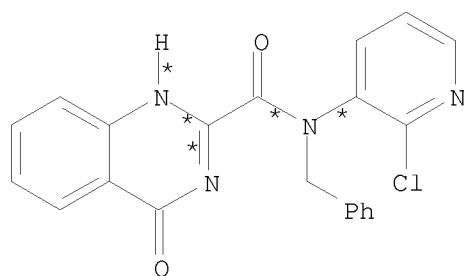
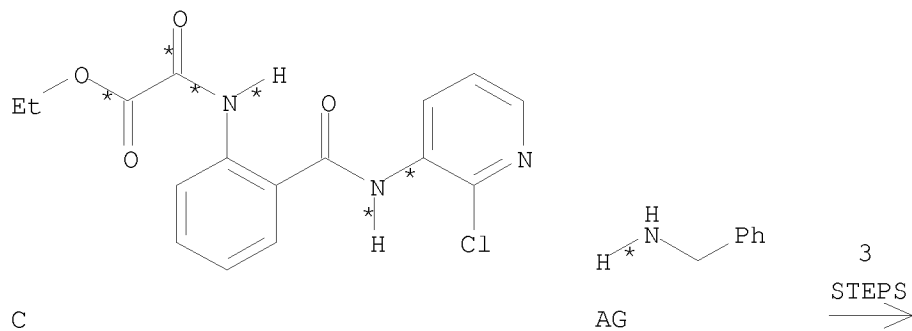
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RGT AJ 304-59-6 Rochelle salt  
SOL 7732-18-5 Water  
CON 0 deg C

PRO AQ 852534-88-4

RX(151) OF 229 COMPOSED OF RX(8), RX(22), RX(43)

RX(151) C + AG ==> BU



BU  
YIELD 85%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3  
SOL 75-09-2 CH2Cl2  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine  
SOL 109-99-9 THF

PRO R 830324-68-0

RX(22) RCT AG 100-46-9

STAGE(1)

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RGT AI 75-24-1 AlMe3  
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 1 hour, room temperature  
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)  
RCT R 830324-68-0  
CON 7 hours, room temperature

STAGE(3)  
RGT AJ 304-59-6 Rochelle salt  
SOL 7732-18-5 Water  
CON 0 deg C

PRO AH 830324-76-0

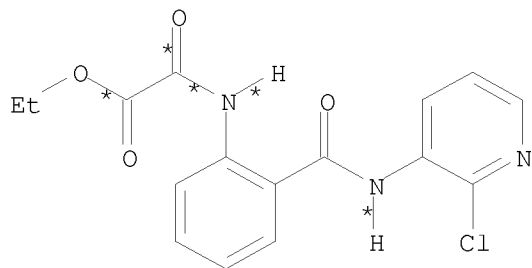
RX(43) RCT AH 830324-76-0

STAGE(1)  
RGT BR 7646-69-7 NaH  
SOL 108-88-3 PhMe  
CON overnight, 80 deg C

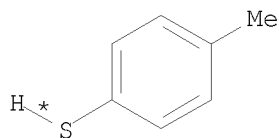
STAGE(2)  
RGT BS 12125-02-9 NH4Cl  
SOL 7732-18-5 Water

PRO BU 830324-81-7  
NTE optimization study

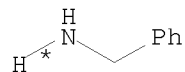
RX(153) OF 229 COMPOSED OF RX(8), RX(38), RX(28)  
RX(153) C + BM + AG ==> AH



C



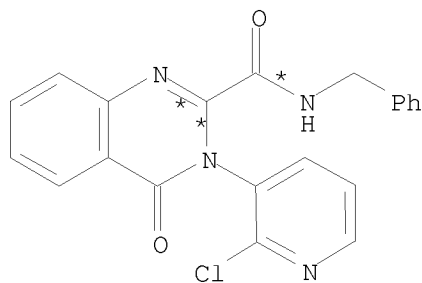
BM



AG

3  
STEPS  
→

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AH  
YIELD 100%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AR 830324-69-1

RX(28) RCT AG 100-46-9, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH<sub>4</sub>OH

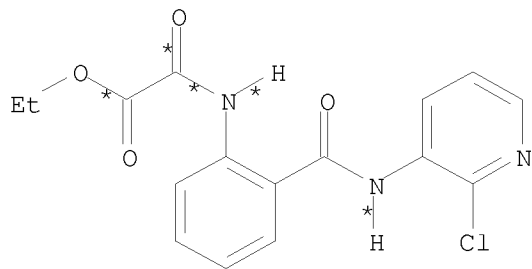
SOL 7732-18-5 Water, 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON 10 minutes, room temperature

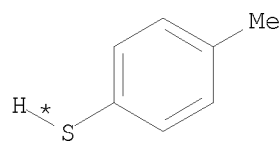
PRO AH 830324-76-0

RX(154) OF 229 COMPOSED OF RX(8), RX(38), RX(30)

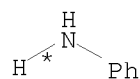
RX(154) C + BM + AX ==> AY



C

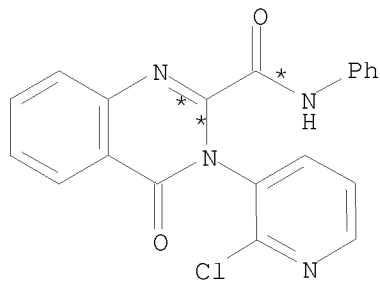


BM



AX

3  
STEPS  
→



AY  
YIELD 100%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)<sub>2</sub>, T 7553-56-2 I<sub>2</sub>, U 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

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PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AR 830324-69-1

RX(30) RCT AX 62-53-3, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

STAGE(2)

RGT AT 1336-21-6 NH4OH

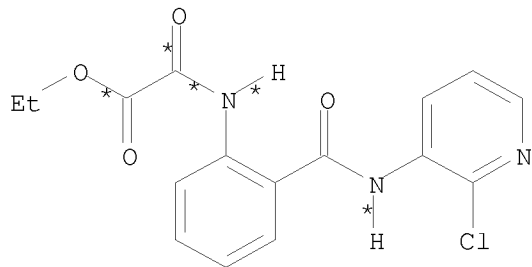
SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

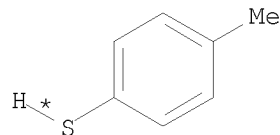
PRO AY 830324-73-7

RX(155) OF 229 COMPOSED OF RX(8), RX(38), RX(33)

RX(155) C + BM + BC ==> BD



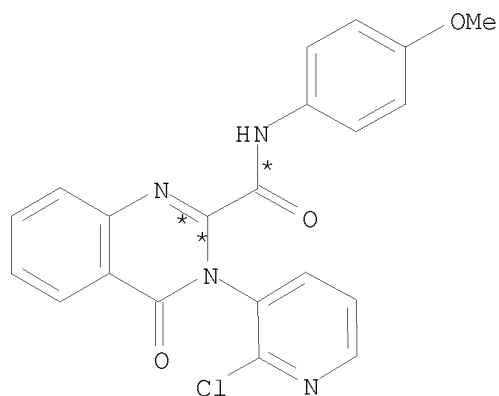
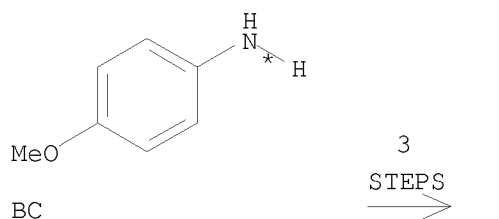
C



BM



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BD  
YIELD 100%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

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STAGE(3)

RGT AJ 304-59-6 Rochelle salt  
SOL 7732-18-5 Water  
CON 0 deg C

PRO AR 830324-69-1

RX(33) RCT BC 104-94-9, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag  
SOL 109-99-9 THF, 108-88-3 PhMe  
CON SUBSTAGE(1) 1.5 hours, 60 deg C  
SUBSTAGE(2) 60 deg C -> room temperature

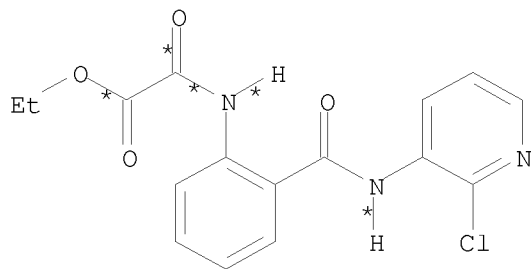
STAGE(2)

RGT AT 1336-21-6 NH4OH  
SOL 7732-18-5 Water, 75-09-2 CH2Cl2  
CON 10 minutes, room temperature

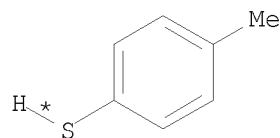
PRO BD 830324-74-8

RX(156) OF 229 COMPOSED OF RX(8), RX(38), RX(34)

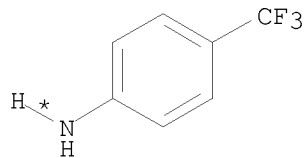
RX(156) C + BM + BE ==> BF



C

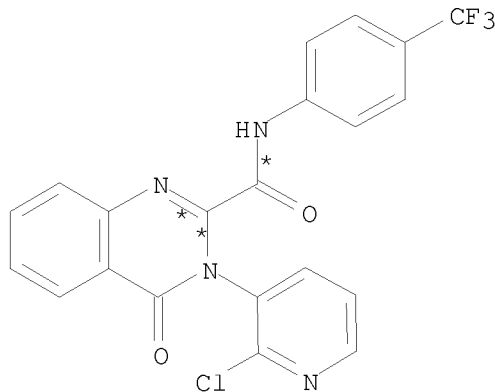


BM



BE

3  
STEPS  
=>



BF  
YIELD 100%

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RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AR 830324-69-1

RX(34) RCT BE 455-14-1, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

STAGE(2)

RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

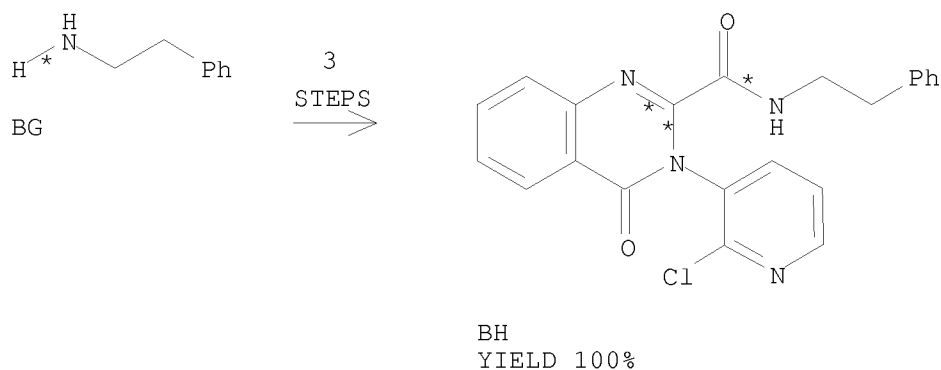
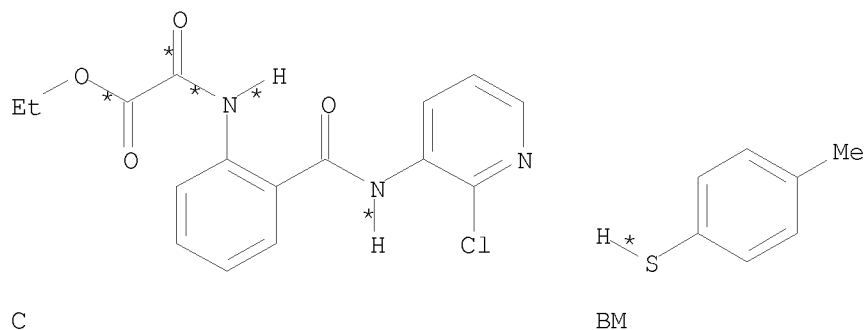
CON 10 minutes, room temperature

PRO BF 830324-75-9

RX(157) OF 229 COMPOSED OF RX(8), RX(38), RX(35)

RX(157) C + BM + BG ==> BH

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RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

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STAGE(3)

RGT AJ 304-59-6 Rochelle salt  
SOL 7732-18-5 Water  
CON 0 deg C

PRO AR 830324-69-1

RX(35) RCT BG 64-04-0, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag  
SOL 109-99-9 THF, 108-88-3 PhMe  
CON SUBSTAGE(1) 1.5 hours, 60 deg C  
SUBSTAGE(2) 60 deg C -> room temperature

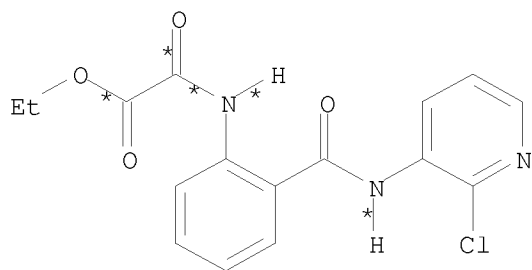
STAGE(2)

RGT AT 1336-21-6 NH4OH  
SOL 7732-18-5 Water, 75-09-2 CH2Cl2  
CON 10 minutes, room temperature

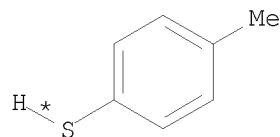
PRO BH 830324-77-1

RX(158) OF 229 COMPOSED OF RX(8), RX(38), RX(37)

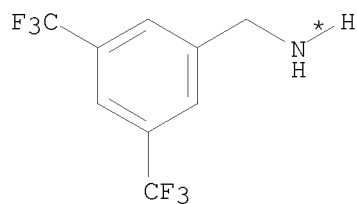
RX(158) C + BM + BK ==> BL



C



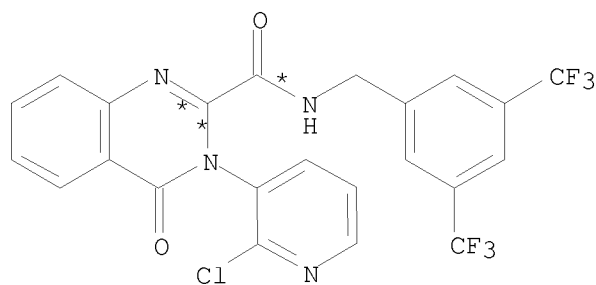
BM



BK

3  
STEPS  
→

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BL  
YIELD 100%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)<sub>2</sub>, T 7553-56-2 I<sub>2</sub>, U 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AR 830324-69-1

RX(37) RCT AR 830324-69-1, BK 85068-29-7

STAGE(1)

RGT AS 2966-50-9 F<sub>3</sub>CCO<sub>2</sub> Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

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## STAGE (2)

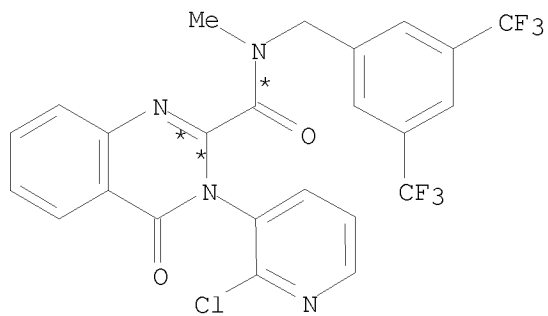
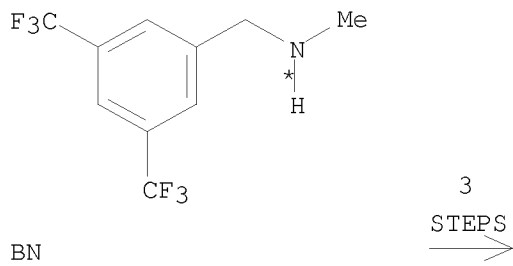
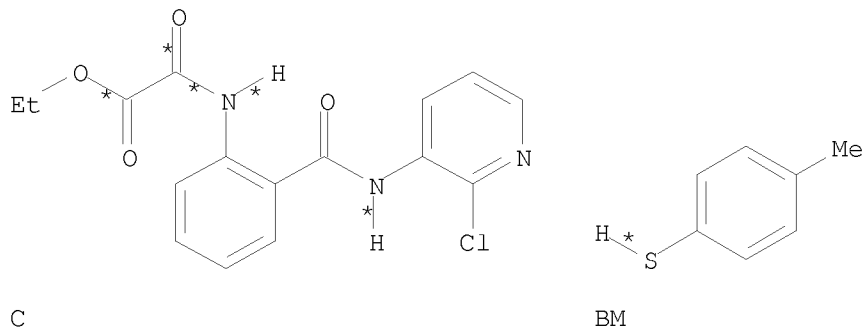
RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2C12

CON 10 minutes, room temperature

PRO BL 830324-70-4

RX(159) OF 229 COMPOSED OF RX(8), RX(38), RX(41)

$$\text{RX}(159) \quad \text{C} + \text{BM} + \text{BN} \implies \text{BO}$$


BO  
YIELD 100%

RX (8) RCT C 830324-66-8

STAGE (1)

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RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3  
SOL 75-09-2 CH2Cl2  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)  
RGT V 123-75-1 Pyrrolidine  
SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)  
RGT AI 75-24-1 AlMe3  
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 30 minutes, room temperature  
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)  
RCT R 830324-68-0  
CON SUBSTAGE(1) 80 minutes, room temperature  
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)  
RGT AJ 304-59-6 Rochelle salt  
SOL 7732-18-5 Water  
CON 0 deg C

PRO AR 830324-69-1

RX(41) RCT AR 830324-69-1, BN 159820-24-3

STAGE(1)  
RGT AS 2966-50-9 F3CCO2 Ag  
SOL 109-99-9 THF, 108-88-3 PhMe  
CON SUBSTAGE(1) 1.5 hours, 60 deg C  
SUBSTAGE(2) 60 deg C -> room temperature

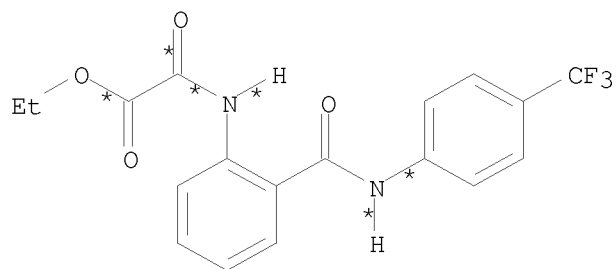
STAGE(2)  
RGT AT 1336-21-6 NH4OH  
SOL 7732-18-5 Water, 75-09-2 CH2Cl2  
CON 10 minutes, room temperature

PRO BO 830324-71-5

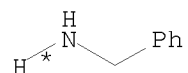
RX(169) OF 229 COMPOSED OF RX(9), RX(23), RX(48)  
RX(169) G + AG ==> BZ



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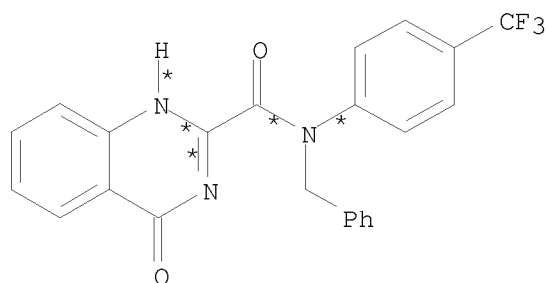


G



AG

3  
STEPS  
→



BZ  
YIELD 95%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO X 361180-29-2

RX(23) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 1 hour, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT X 361180-29-2

CON 7 hours, room temperature

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STAGE(3)

RGT AJ 304-59-6 Rochelle salt  
SOL 7732-18-5 Water  
CON 0 deg C

PRO AM 830324-84-0

RX(48) RCT AM 830324-84-0

STAGE(1)

RGT BR 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 0 deg C -> room temperature  
SUBSTAGE(2) 1 hour, room temperature

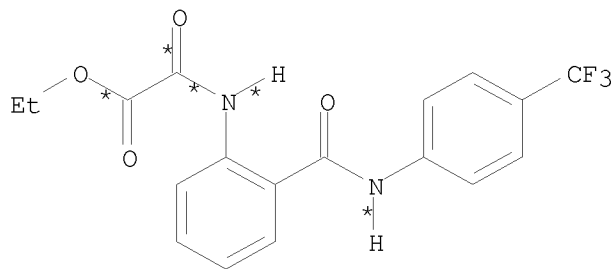
STAGE(2)

RGT BS 12125-02-9 NH4Cl  
SOL 7732-18-5 Water  
CON 0 deg C

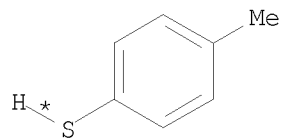
PRO BZ 830324-91-9

RX(170) OF 229 COMPOSED OF RX(9), RX(39), RX(31)

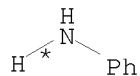
RX(170) G + BM + AX ==> BA



G



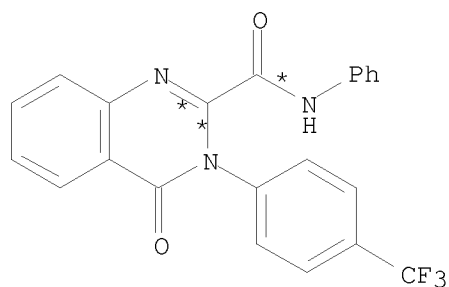
BM



AX

3  
STEPS  
→

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BA  
YIELD 81%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO X 361180-29-2

RX(39) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT X 361180-29-2

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AZ 852534-84-0

RX(31) RCT AX 62-53-3, AZ 852534-84-0

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

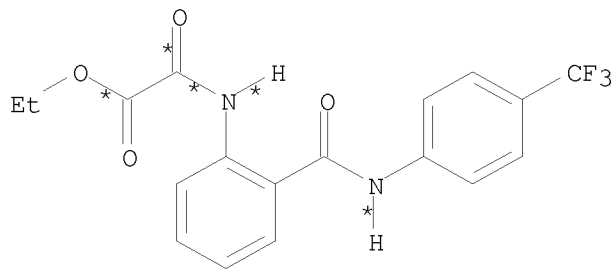
SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

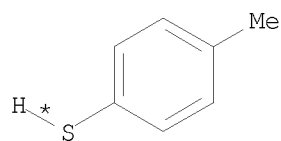
PRO BA 830324-83-9

RX(171) OF 229 COMPOSED OF RX(9), RX(39), RX(36)

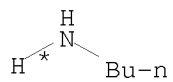
RX(171) G + BM + BI ==> BJ



G

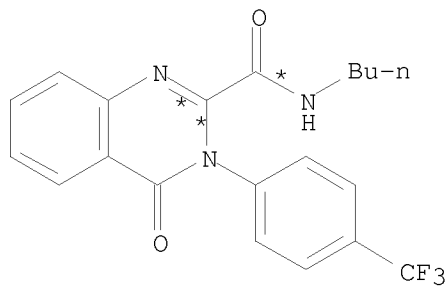


BM



BI

3  
STEPS  
→



BJ

YIELD 96%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

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SOL 109-99-9 THF

PRO X 361180-29-2

RX(39) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT X 361180-29-2

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AZ 852534-84-0

RX(36) RCT BI 109-73-9, AZ 852534-84-0

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

STAGE(2)

RGT AT 1336-21-6 NH4OH

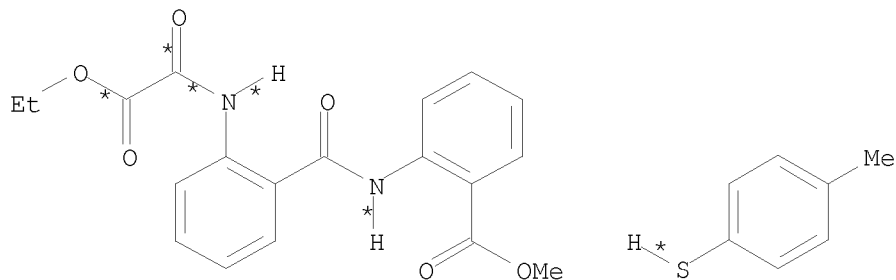
SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

PRO BJ 830324-85-1

RX(175) OF 229 COMPOSED OF RX(10), RX(40), RX(29)

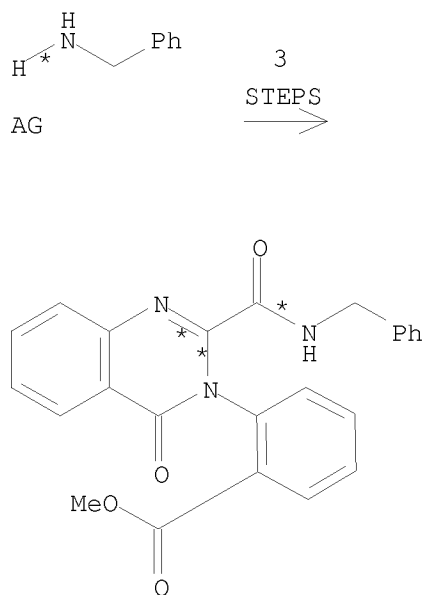
RX(175) I + BM + AG ==> AW



I

BM

10/ 562,112



YIELD 100%

RX(10) RCT I 852534-80-6

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO Y 852534-83-9

RX(40) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT Y 852534-83-9

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

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PRO AV 852534-85-1

RX(29) RCT AG 100-46-9, AV 852534-85-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

STAGE(2)

RGT AT 1336-21-6 NH4OH

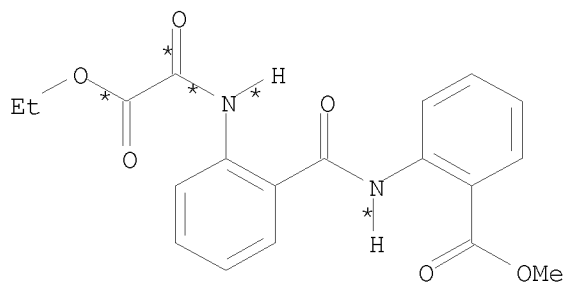
SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

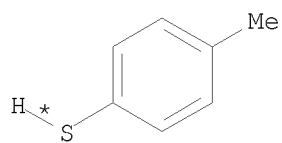
PRO AW 830324-89-5

RX(176) OF 229 COMPOSED OF RX(10), RX(40), RX(32)

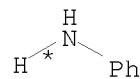
RX(176) I + BM + AX ==> BB



I

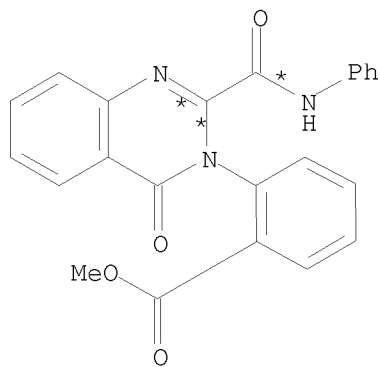


BM



AX

3  
STEPS  
→



BB

YIELD 87%

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RX(10) RCT I 852534-80-6

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO Y 852534-83-9

RX(40) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT Y 852534-83-9

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AV 852534-85-1

RX(32) RCT AX 62-53-3, AV 852534-85-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

STAGE(2)

RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

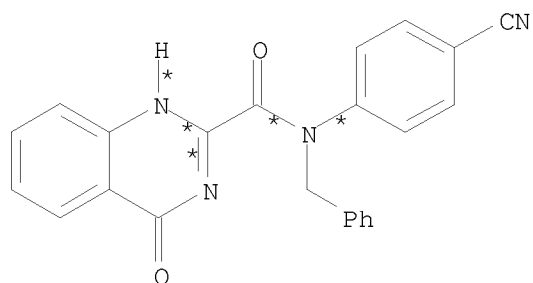
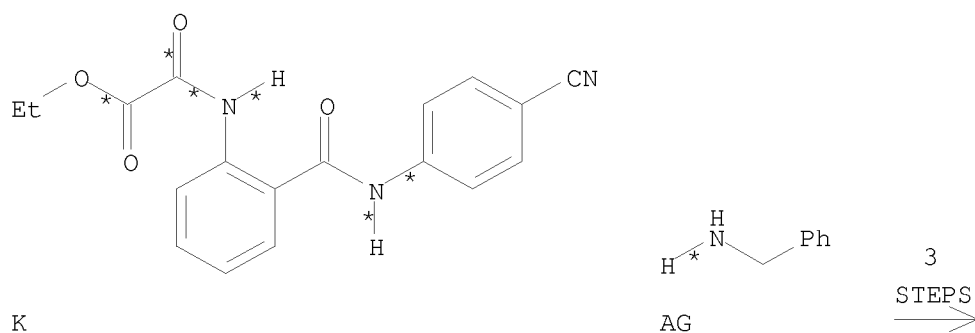
PRO BB 830324-87-3

RX(179) OF 229 COMPOSED OF RX(11), RX(24), RX(53)

RX(179) K + AG ==> CE



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CE  
YIELD 95%

RX(11) RCT K 852534-81-7

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO Z 830325-00-3

RX(24) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 1 hour, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT Z 830325-00-3

CON 7 hours, room temperature

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STAGE(3)

RGT AJ 304-59-6 Rochelle salt  
SOL 7732-18-5 Water  
CON 0 deg C

PRO AN 830324-86-2

RX(53) RCT AN 830324-86-2

STAGE(1)

RGT BR 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 0 deg C -> room temperature  
SUBSTAGE(2) 1 hour, room temperature

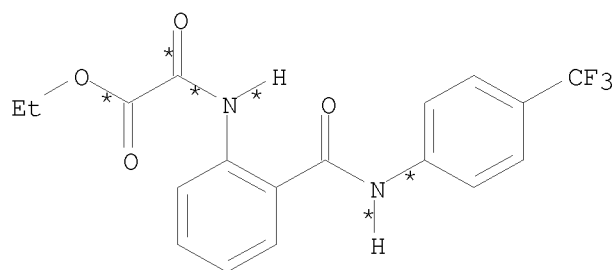
STAGE(2)

RGT BS 12125-02-9 NH4Cl  
SOL 7732-18-5 Water  
CON 0 deg C

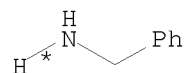
PRO CE 830324-93-1

RX(182) OF 229 COMPOSED OF RX(9), RX(23), RX(48), RX(57)

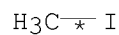
RX(182) G + AG + BP ==> CK



G



AG

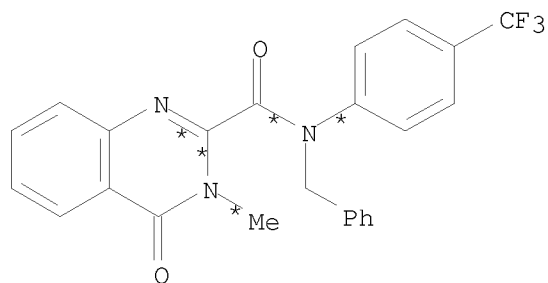


BP

4

STEPS  
=>

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CK  
YIELD 92%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)<sub>2</sub>, T 7553-56-2 I<sub>2</sub>, U 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO X 361180-29-2

RX(23) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 1 hour, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT X 361180-29-2

CON 7 hours, room temperature

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AM 830324-84-0

RX(48) RCT AM 830324-84-0

STAGE(1)

RGT BR 7646-69-7 NaH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

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RGT BS 12125-02-9 NH4Cl  
SOL 7732-18-5 Water  
CON 0 deg C

PRO BZ 830324-91-9

RX(57) RCT BZ 830324-91-9, BP 74-88-4

STAGE(1)

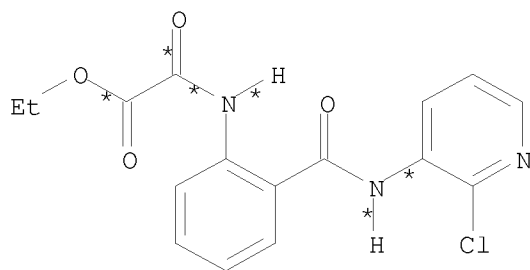
RGT BR 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 50 minutes, room temperature  
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

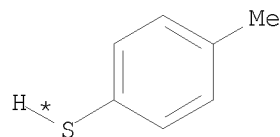
RGT BS 12125-02-9 NH4Cl  
SOL 7732-18-5 Water  
CON 0 deg C

PRO CK 830324-99-7

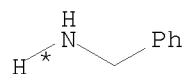
RX(194) OF 229 COMPOSED OF RX(8), RX(38), RX(28), RX(43)  
RX(194) C + BM + AG ==> BU



C



BM

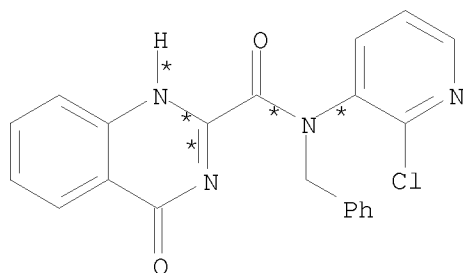


AG

4

STEPS  
→

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BU  
YIELD 85%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)<sub>2</sub>, T 7553-56-2 I<sub>2</sub>, U 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AR 830324-69-1

RX(28) RCT AG 100-46-9, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F<sub>3</sub>CCO<sub>2</sub> Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

PRO AH 830324-76-0

RX(43) RCT AH 830324-76-0

STAGE(1)

RGT BR 7646-69-7 NaH

SOL 108-88-3 PhMe

CON overnight, 80 deg C

STAGE(2)

RGT BS 12125-02-9 NH4Cl

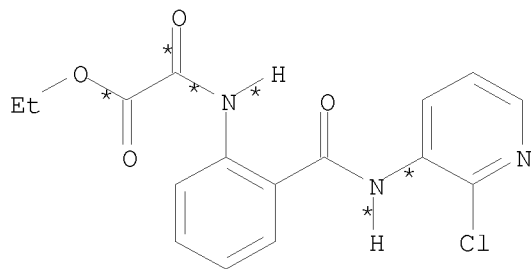
SOL 7732-18-5 Water

PRO BU 830324-81-7

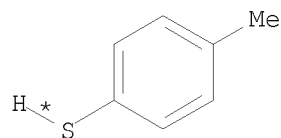
NTE optimization study

RX(196) OF 229 COMPOSED OF RX(8), RX(38), RX(30), RX(44)

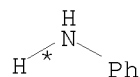
RX(196) C + BM + AX ==> BV



C



BM

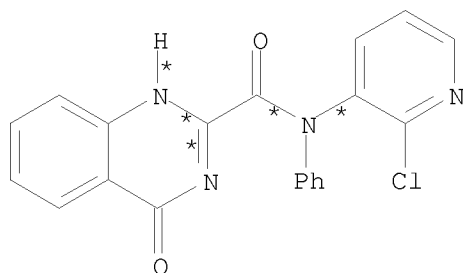


AX

4

STEPS  
=>

10/ 562,112



BV  
YIELD 88%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)<sub>2</sub>, T 7553-56-2 I<sub>2</sub>, U 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AR 830324-69-1

RX(30) RCT AX 62-53-3, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F<sub>3</sub>CCO<sub>2</sub> Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

PRO AY 830324-73-7

RX(44) RCT AY 830324-73-7

STAGE(1)

RGT BR 7646-69-7 NaH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

RGT BS 12125-02-9 NH4Cl

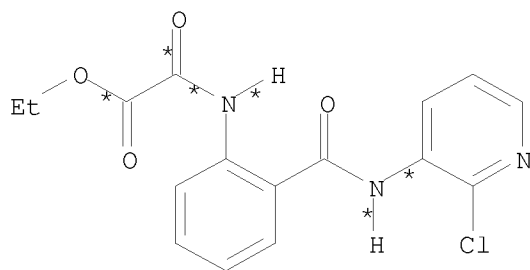
SOL 7732-18-5 Water

CON 0 deg C

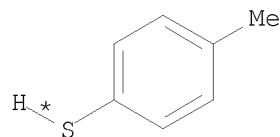
PRO BV 830324-78-2

RX(198) OF 229 COMPOSED OF RX(8), RX(38), RX(33), RX(45)

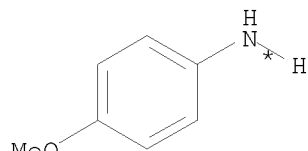
RX(198) C + BM + BC ==> BW



C



BM

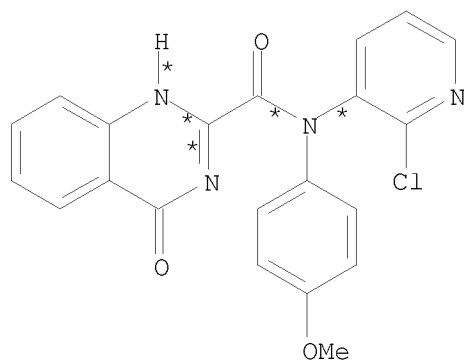


BC

4  
STEPS  
→



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BW  
YIELD 87%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)<sub>2</sub>, T 7553-56-2 I<sub>2</sub>, U 603-35-0 PPh<sub>3</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine  
SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe<sub>3</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 110-54-3 Hexane  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 30 minutes, room temperature  
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0  
CON SUBSTAGE(1) 80 minutes, room temperature  
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt  
SOL 7732-18-5 Water  
CON 0 deg C

PRO AR 830324-69-1

RX(33) RCT BC 104-94-9, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F<sub>3</sub>CCO<sub>2</sub> Ag  
SOL 109-99-9 THF, 108-88-3 PhMe

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CON SUBSTAGE(1) 1.5 hours, 60 deg C  
SUBSTAGE(2) 60 deg C -> room temperature

STAGE(2)

RGT AT 1336-21-6 NH4OH  
SOL 7732-18-5 Water, 75-09-2 CH2Cl2  
CON 10 minutes, room temperature

PRO BD 830324-74-8

RX(45) RCT BD 830324-74-8

STAGE(1)

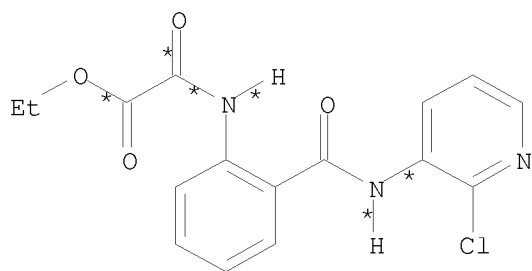
RGT BR 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 0 deg C -> room temperature  
SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

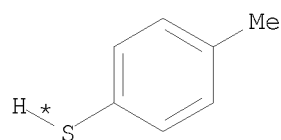
RGT BS 12125-02-9 NH4Cl  
SOL 7732-18-5 Water  
CON 0 deg C

PRO BW 830324-79-3

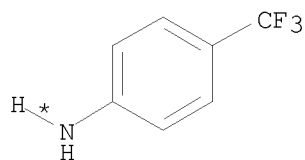
RX(200) OF 229 COMPOSED OF RX(8), RX(38), RX(34), RX(46)  
RX(200) C + BM + BE ==> BX



C



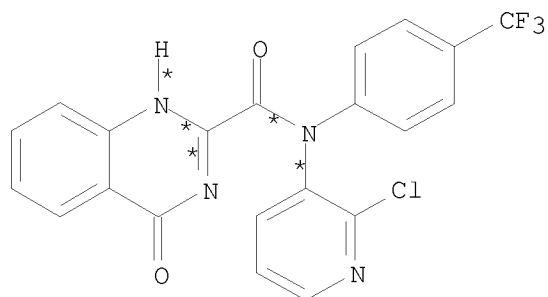
BM



BE

4  
STEPS  
→

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BX  
YIELD 100%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)<sub>2</sub>, T 7553-56-2 I<sub>2</sub>, U 603-35-0 PPh<sub>3</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine  
SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe<sub>3</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 110-54-3 Hexane  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 30 minutes, room temperature  
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0  
CON SUBSTAGE(1) 80 minutes, room temperature  
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt  
SOL 7732-18-5 Water  
CON 0 deg C

PRO AR 830324-69-1

RX(34) RCT BE 455-14-1, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F<sub>3</sub>CCO<sub>2</sub> Ag  
SOL 109-99-9 THF, 108-88-3 PhMe  
CON SUBSTAGE(1) 1.5 hours, 60 deg C  
SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

PRO BF 830324-75-9

RX(46) RCT BF 830324-75-9

STAGE(1)

RGT BR 7646-69-7 NaH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

RGT BS 12125-02-9 NH4Cl

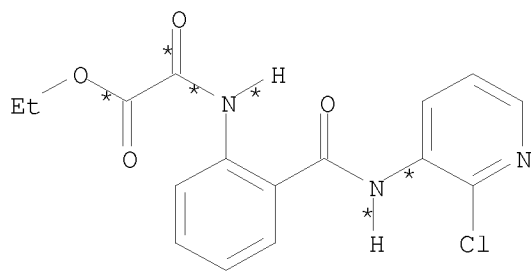
SOL 7732-18-5 Water

CON 0 deg C

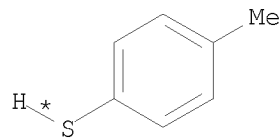
PRO BX 830324-80-6

RX(202) OF 229 COMPOSED OF RX(8), RX(38), RX(35), RX(47)

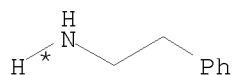
RX(202) C + BM + BG ==> BY



C



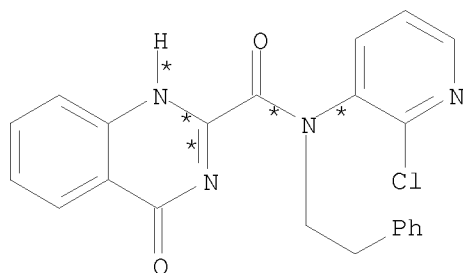
BM



BG

4  
STEPS  
→

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BY  
YIELD 63%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AR 830324-69-1

RX(35) RCT BG 64-04-0, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

PRO BH 830324-77-1

RX(47) RCT BH 830324-77-1

STAGE(1)

RGT BR 7646-69-7 NaH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

RGT BS 12125-02-9 NH4Cl

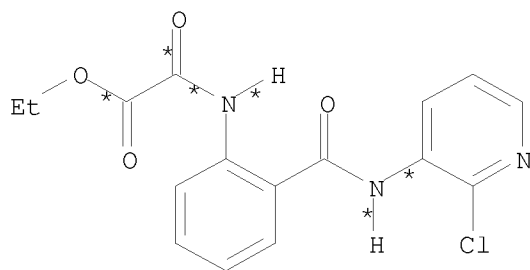
SOL 7732-18-5 Water

CON 0 deg C

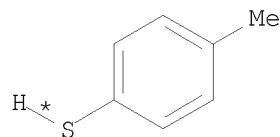
PRO BY 830324-82-8

RX(204) OF 229 COMPOSED OF RX(8), RX(38), RX(37), RX(42)

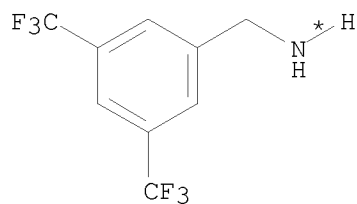
RX(204) C + BM + BK + BP ==> BQ



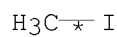
C



BM



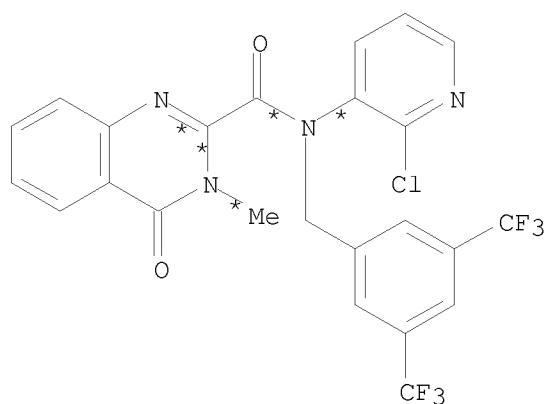
BK



BP

4  
STEPS  
→

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BQ  
YIELD 81%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)<sub>2</sub>, T 7553-56-2 I<sub>2</sub>, U 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AR 830324-69-1

RX(37) RCT AR 830324-69-1, BK 85068-29-7

STAGE(1)

RGT AS 2966-50-9 F<sub>3</sub>CCO<sub>2</sub> Ag

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SOL 109-99-9 THF, 108-88-3 PhMe  
CON SUBSTAGE(1) 1.5 hours, 60 deg C  
SUBSTAGE(2) 60 deg C -> room temperature

STAGE(2)

RGT AT 1336-21-6 NH4OH  
SOL 7732-18-5 Water, 75-09-2 CH2Cl2  
CON 10 minutes, room temperature

PRO BL 830324-70-4

RX(42) RCT BL 830324-70-4

STAGE(1)

RGT BR 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 0 deg C -> room temperature  
SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

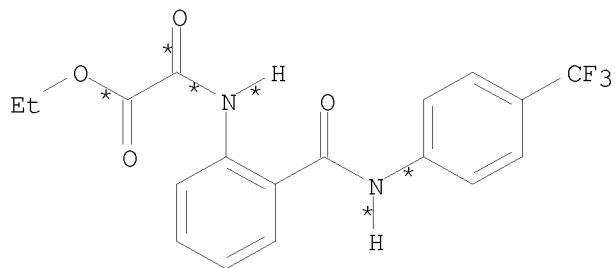
RCT BP 74-88-4  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 1 hour, room temperature

STAGE(3)

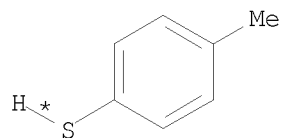
RGT BS 12125-02-9 NH4Cl  
SOL 7732-18-5 Water  
CON 0 deg C

PRO BQ 830324-72-6

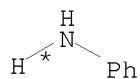
RX(207) OF 229 COMPOSED OF RX(9), RX(39), RX(31), RX(49)  
RX(207) G + BM + AX ==> CA



G



BM

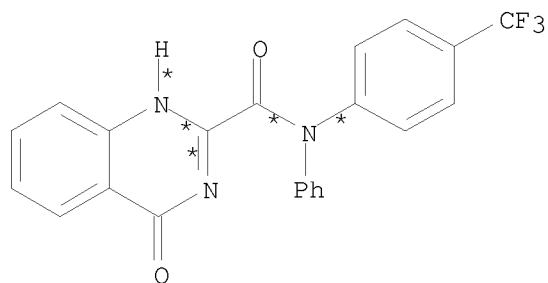


AX

4  
STEPS  
→



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CA  
YIELD 85%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)<sub>2</sub>, T 7553-56-2 I<sub>2</sub>, U 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO X 361180-29-2

RX(39) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT X 361180-29-2

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AZ 852534-84-0

RX(31) RCT AX 62-53-3, AZ 852534-84-0

STAGE(1)

RGT AS 2966-50-9 F<sub>3</sub>CCO<sub>2</sub> Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

PRO BA 830324-83-9

RX(49) RCT BA 830324-83-9

STAGE(1)

RGT BR 7646-69-7 NaH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

RGT BS 12125-02-9 NH4Cl

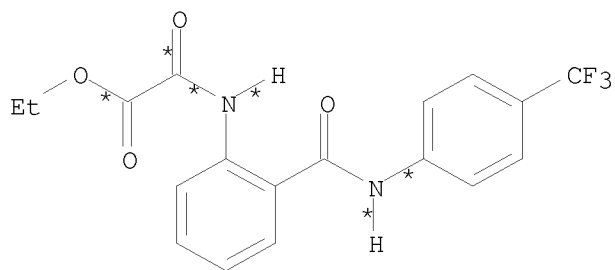
SOL 7732-18-5 Water

CON 0 deg C

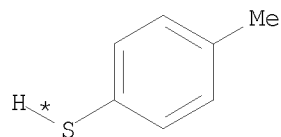
PRO CA 830324-90-8

RX(208) OF 229 COMPOSED OF RX(9), RX(39), RX(36), RX(50)

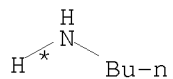
RX(208) G + BM + BI ==> CB



G



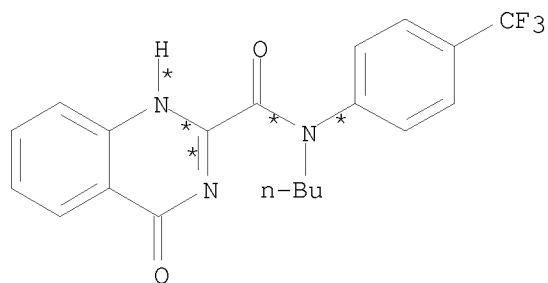
BM



BI

4  
STEPS  
→

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CB  
YIELD 100%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)<sub>2</sub>, T 7553-56-2 I<sub>2</sub>, U 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO X 361180-29-2

RX(39) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT X 361180-29-2

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AZ 852534-84-0

RX(36) RCT BI 109-73-9, AZ 852534-84-0

STAGE(1)

RGT AS 2966-50-9 F<sub>3</sub>CCO<sub>2</sub> Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

PRO BJ 830324-85-1

RX(50) RCT BJ 830324-85-1

STAGE(1)

RGT BR 7646-69-7 NaH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

RGT BS 12125-02-9 NH4Cl

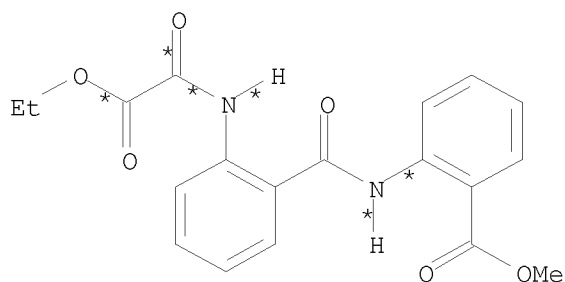
SOL 7732-18-5 Water

CON 0 deg C

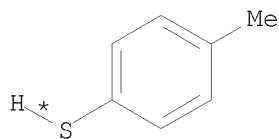
PRO CB 830324-92-0

RX(211) OF 229 COMPOSED OF RX(10), RX(40), RX(29), RX(51)

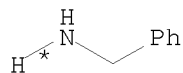
RX(211) I + BM + AG ==> CC



I



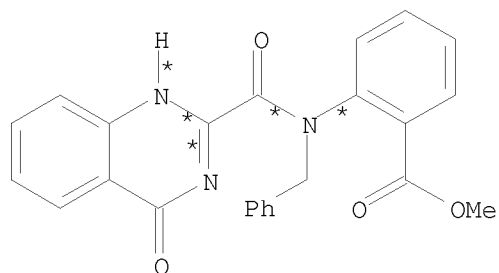
BM



AG

4  
STEPS  
→

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CC  
YIELD 100%

RX(10) RCT I 852534-80-6

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO Y 852534-83-9

RX(40) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT Y 852534-83-9

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AV 852534-85-1

RX(29) RCT AG 100-46-9, AV 852534-85-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

PRO AW 830324-89-5

RX(51) RCT AW 830324-89-5

STAGE(1)

RGT BR 7646-69-7 NaH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

RGT BS 12125-02-9 NH4Cl

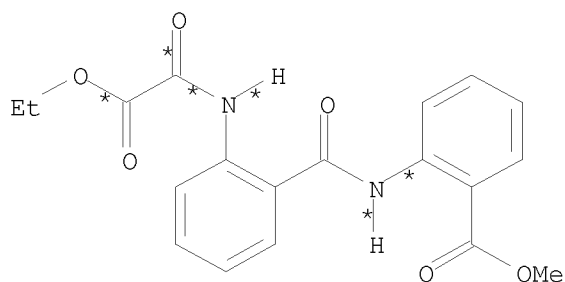
SOL 7732-18-5 Water

CON 0 deg C

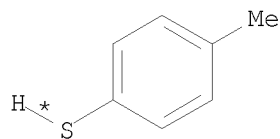
PRO CC 830324-96-4

RX(212) OF 229 COMPOSED OF RX(10), RX(40), RX(32), RX(52)

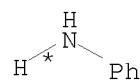
RX(212) I + BM + AX ==> CD



I



BM



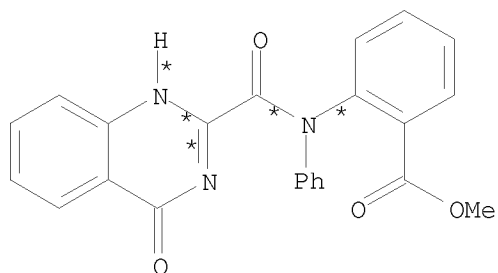
AX

4

STEPS



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CD  
YIELD 72%

RX(10) RCT I 852534-80-6

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)<sub>2</sub>, T 7553-56-2 I<sub>2</sub>, U 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO Y 852534-83-9

RX(40) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT Y 852534-83-9

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AV 852534-85-1

RX(32) RCT AX 62-53-3, AV 852534-85-1

STAGE(1)

RGT AS 2966-50-9 F<sub>3</sub>CCO<sub>2</sub> Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH  
SOL 7732-18-5 Water, 75-09-2 CH2Cl2  
CON 10 minutes, room temperature

PRO BB 830324-87-3

RX(52) RCT BB 830324-87-3

STAGE(1)

RGT BR 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 0 deg C -> room temperature  
SUBSTAGE(2) 1 hour, room temperature

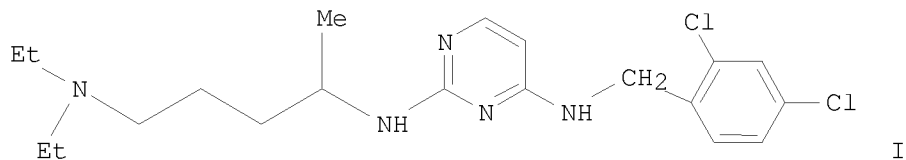
STAGE(2)

RGT BS 12125-02-9 NH4Cl  
SOL 7732-18-5 Water  
CON 0 deg C

PRO CD 830324-94-2

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 51 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 143:336 CASREACT  
TITLE: Identification of chemokine receptor CCR4 antagonist  
AUTHOR(S): Purandare, Ashok V.; Gao, Aiming; Wan, Honghe;  
Somerville, John; Burke, Christine; Seachord, Carrie;  
Vaccaro, Wayne; Wityak, John; Poss, Michael A.  
CORPORATE SOURCE: Bristol-Myers Squibb Pharmaceutical Research  
Institute, Princeton, NJ, 08543, USA  
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005),  
15(10), 2669-2672  
CODEN: BMCLE8; ISSN: 0960-894X  
PUBLISHER: Elsevier B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

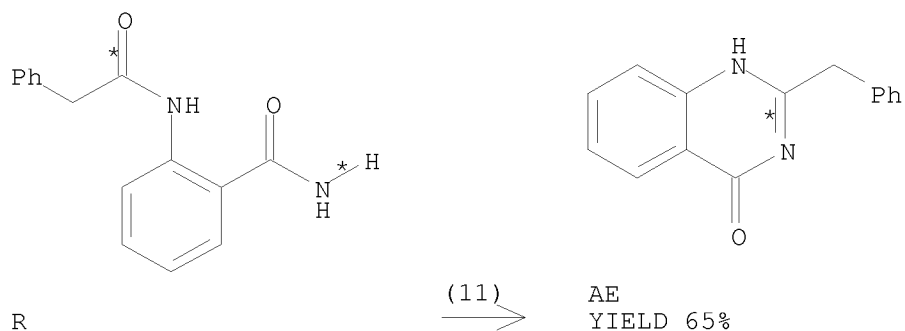


AB The present study reports the identification and hits to leads optimization of chemokine receptor CCR4 antagonists. Compound I is a high affinity, noncytotoxic antagonist of CCR4 that blocks the functional activity mediated by the receptor.



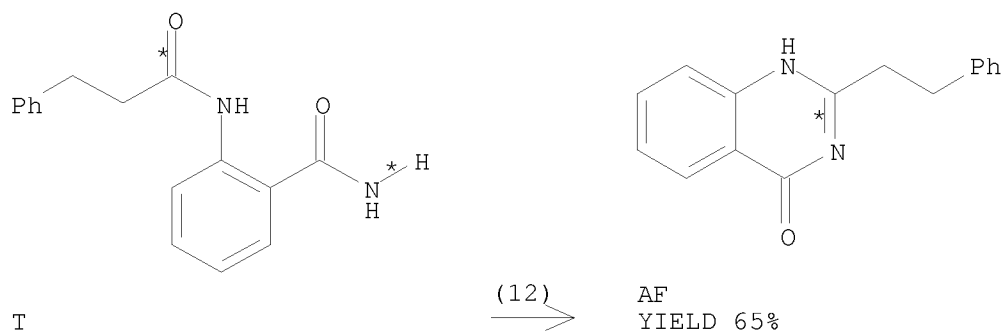
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RX(11) OF 68      ...R ==> AE...



RX(11)      RCT    R 52910-86-8  
              RGT    AB 141-52-6 NaOEt, AC 7722-84-1 H2O2  
              PRO    AE 4765-56-4  
              CON    room temperature

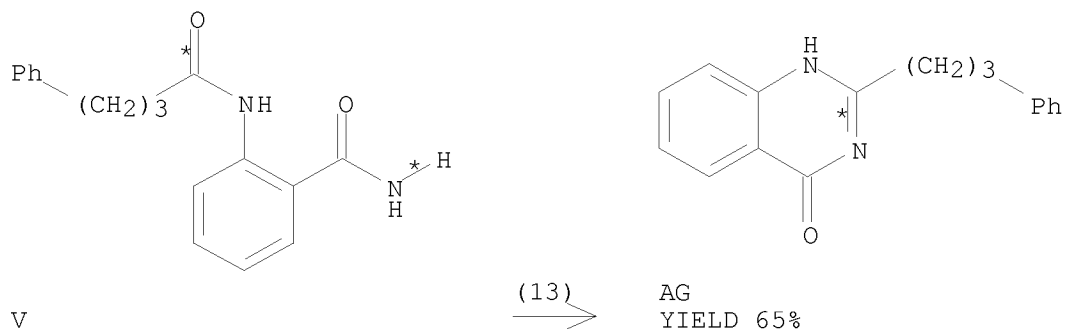
RX(12) OF 68      ...T ==> AF...



RX(12)      RCT    T 313382-30-8  
              RGT    AB 141-52-6 NaOEt, AC 7722-84-1 H2O2  
              PRO    AF 4765-57-5  
              CON    room temperature

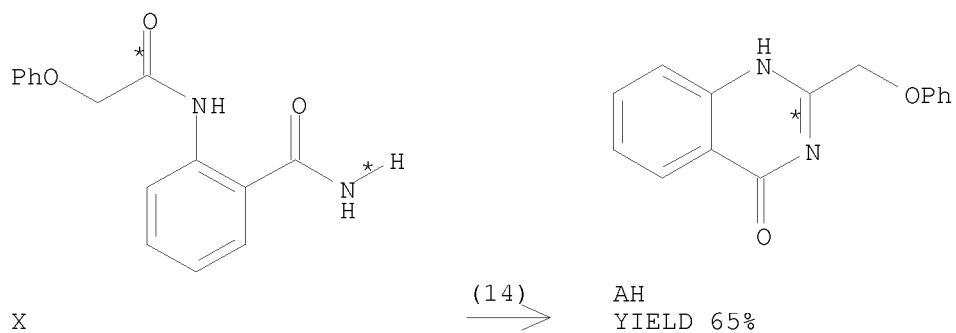
RX(13) OF 68      ...V ==> AG...

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RX(13) RCT V 430453-70-6  
RGT AB 141-52-6 NaOEt, AC 7722-84-1 H2O2  
PRO AG 852460-38-9  
CON room temperature

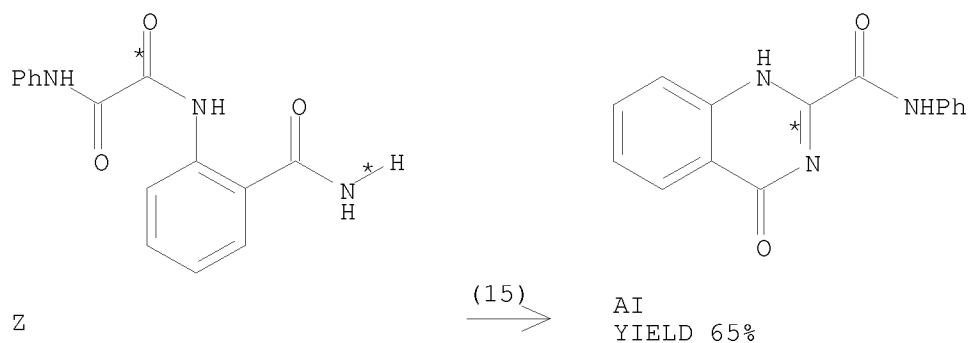
RX(14) OF 68 ...X ==> AH...



RX(14) RCT X 52910-87-9  
RGT AB 141-52-6 NaOEt, AC 7722-84-1 H2O2  
PRO AH 100880-66-8  
CON room temperature

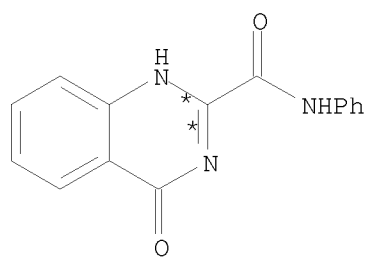
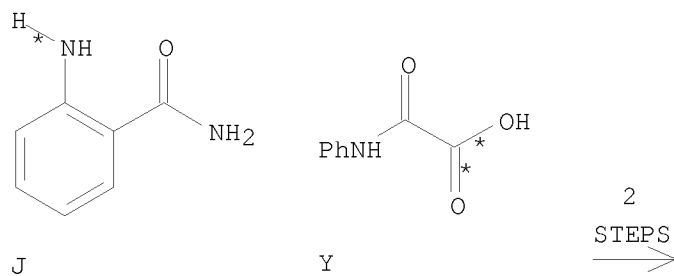
RX(15) OF 68 ...Z ==> AI...

10/ 562,112



RX(15) RCT Z 852460-37-8  
RGT AB 141-52-6 NaOEt, AC 7722-84-1 H2O2  
PRO AI 118372-87-5  
CON room temperature

RX(52) OF 68 COMPOSED OF RX(8), RX(15)  
RX(52) J + Y ==> AI



AI  
YIELD 65%

RX(8) RCT J 88-68-6, Y 500-72-1  
RGT M 25952-53-8 EDAP  
PRO Z 852460-37-8  
SOL 75-09-2 CH2Cl2  
CON room temperature

RX(15) RCT Z 852460-37-8

10/ 562,112

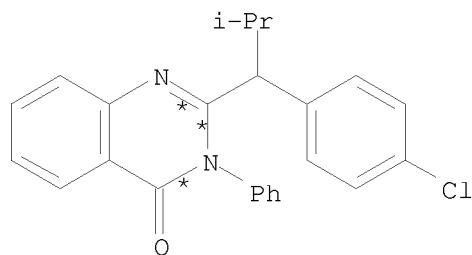
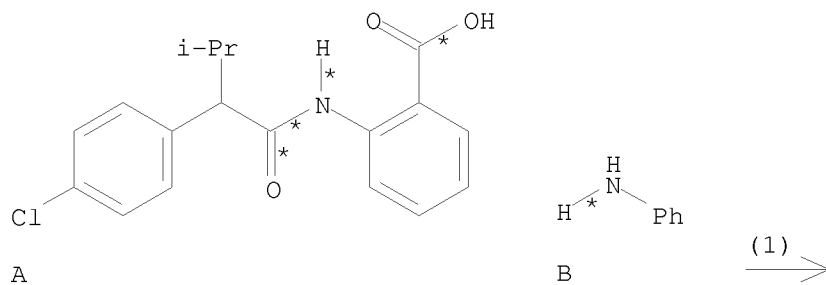
RGT AB 141-52-6 NaOEt, AC 7722-84-1 H2O2  
PRO AI 118372-87-5  
CON room temperature

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 52 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 142:447174 CASREACT  
TITLE: Synthesis and antimicrobial activity of  
2-[1-(4-chlorophenyl)-2-methylpropyl]-3-arylquinazolin-  
4(3H)-ones  
AUTHOR(S): Radadia, V. R.; Purohit, D. M.; Patolia, V. N.  
CORPORATE SOURCE: India  
SOURCE: Indian Journal of Heterocyclic Chemistry (2004),  
14(2), 153-154  
CODEN: IJCHEI; ISSN: 0971-1627  
PUBLISHER: Prof. R. S. Varma  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The title compds. were prepared by the chemoselective cyclocondensation of  
2-[2-(4-chlorophenyl)-3-methylbutanoylamino]benzoic acid (I) with  
arylamines. Compound I was prepared by the amidation of anthranilic acid with  
2-(4-chlorophenyl)-3-methylbutanoyl chloride. Antimicrobial activities of  
varying degree was exhibited by all the compds. prepared

RX(1) OF 33 ...A + B ==> C

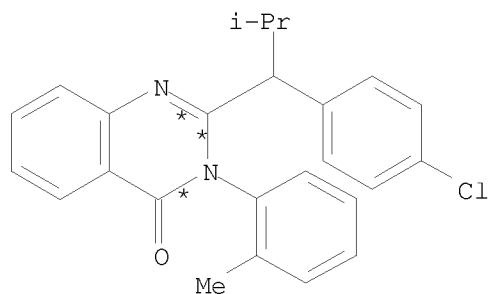
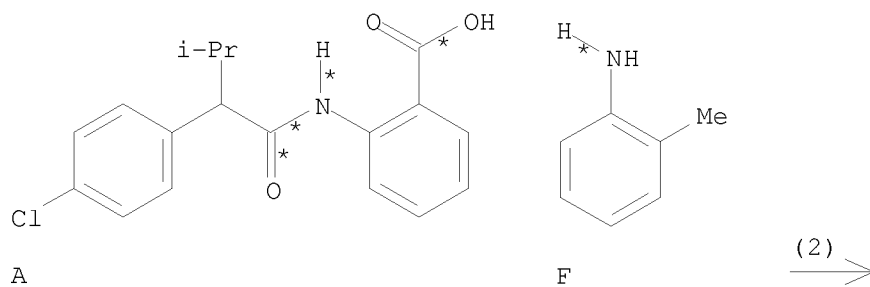


C  
YIELD 75%

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RX(1)        RCT    A 851191-19-0, B 62-53-3  
              RGT    D 110-86-1 Pyridine  
              PRO    C 851191-03-2  
              SOL    64-17-5 EtOH  
              CON    4 hours, reflux  
              NTE    chemoselective

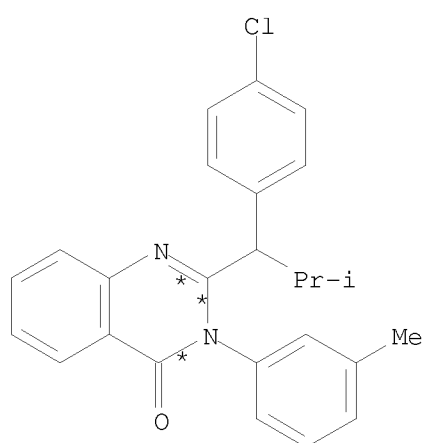
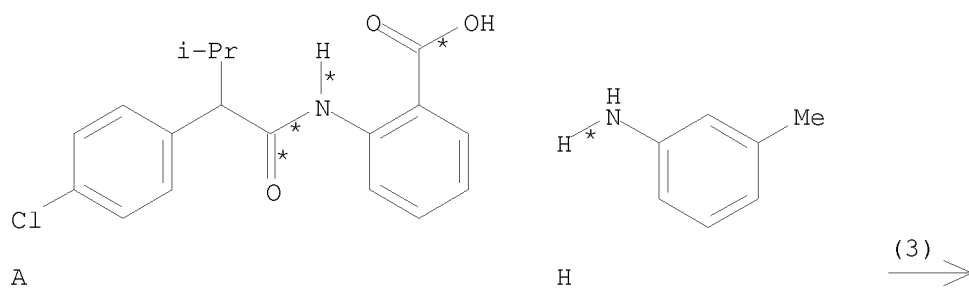
RX(2) OF 33        ...A + F ==> G



G  
YIELD 60%

RX(2)        RCT    A 851191-19-0, F 95-53-4  
              RGT    D 110-86-1 Pyridine  
              PRO    G 851191-04-3  
              SOL    64-17-5 EtOH  
              CON    4 hours, reflux  
              NTE    chemoselective

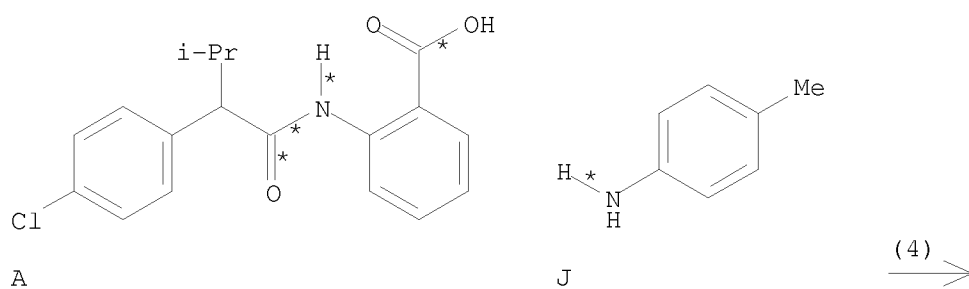
RX(3) OF 33        ...A + H ==> I



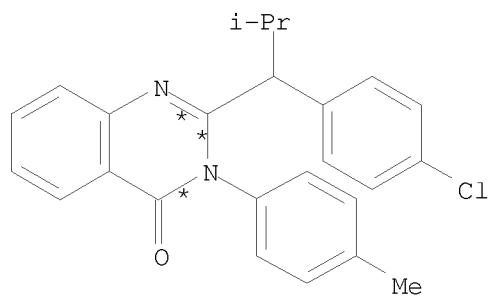
I  
YIELD 66%

RX(3)      RCT    A 851191-19-0, H 108-44-1  
              RGT    D 110-86-1 Pyridine  
              PRO    I 851191-05-4  
              SOL    64-17-5 EtOH  
              CON    4 hours, reflux  
              NTE    chemoselective

RX(4) OF 33      ...A + J  $\implies$  K



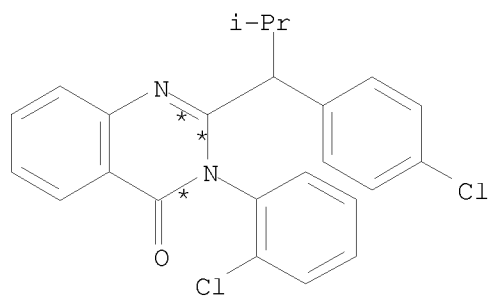
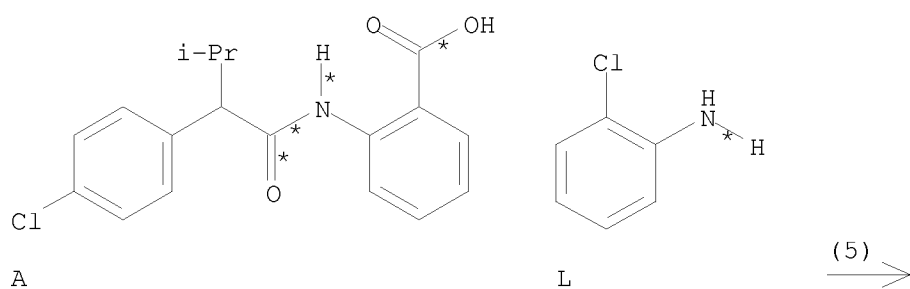
10/ 562,112



K  
YIELD 75%

RX(4)        RCT    A 851191-19-0, J 106-49-0  
              RGT    D 110-86-1 Pyridine  
              PRO    K 851191-06-5  
              SOL    64-17-5 EtOH  
              CON    4 hours, reflux  
              NTE    chemoselective

RX(5) OF 33        ...A + L ==> M



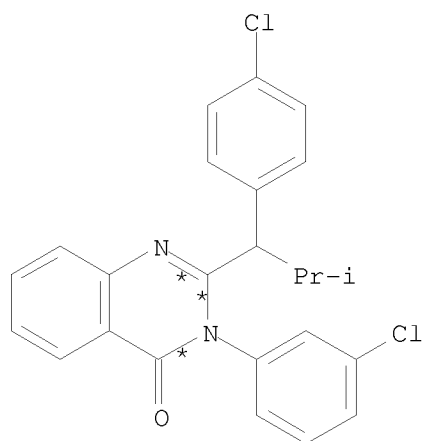
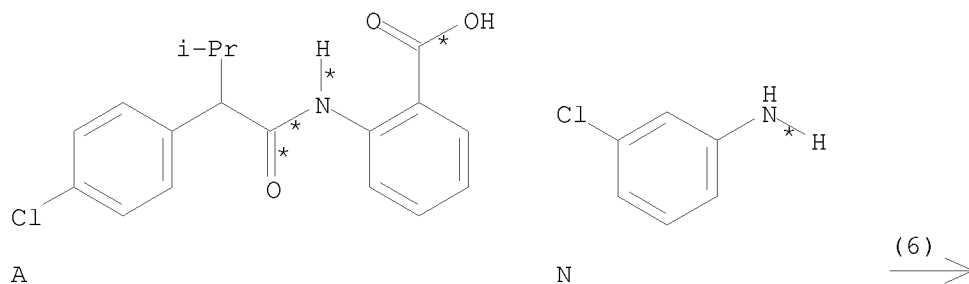
M  
YIELD 65%

RX(5)        RCT    A 851191-19-0, L 95-51-2  
              RGT    D 110-86-1 Pyridine  
              PRO    M 851191-07-6

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SOL 64-17-5 EtOH  
CON 4 hours, reflux  
NTE chemoselective

RX(6) OF 33 ...A + N ==> O

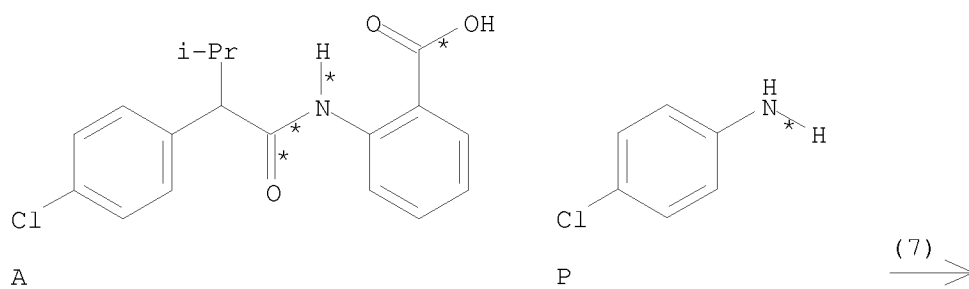


O  
YIELD 70%

RX(6) RCT A 851191-19-0, N 108-42-9  
RGT D 110-86-1 Pyridine  
PRO O 851191-08-7  
SOL 64-17-5 EtOH  
CON 4 hours, reflux  
NTE chemoselective

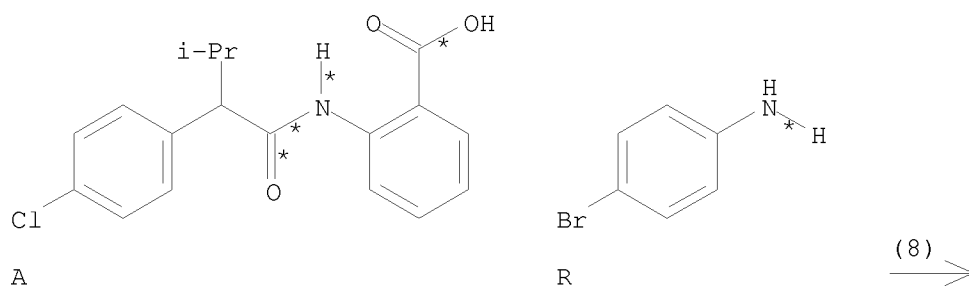
RX(7) OF 33 ...A + P ==> Q



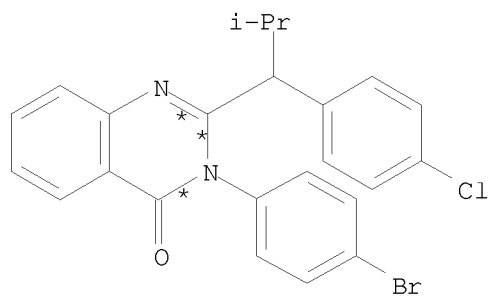


RX(7)      RCT    A 851191-19-0, P 106-47-8  
 RGT    D 110-86-1 Pyridine  
 PRO    Q 851191-09-8  
 SOL    64-17-5 EtOH  
 CON    4 hours, reflux  
 NTE    chemoselective

RX(8) OF 33      ...A + R ==> S



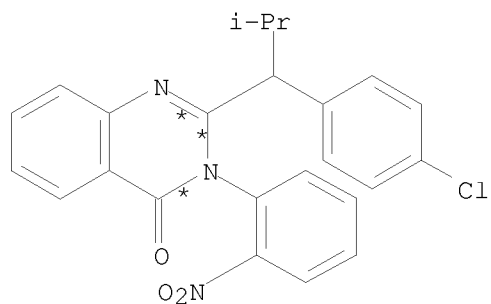
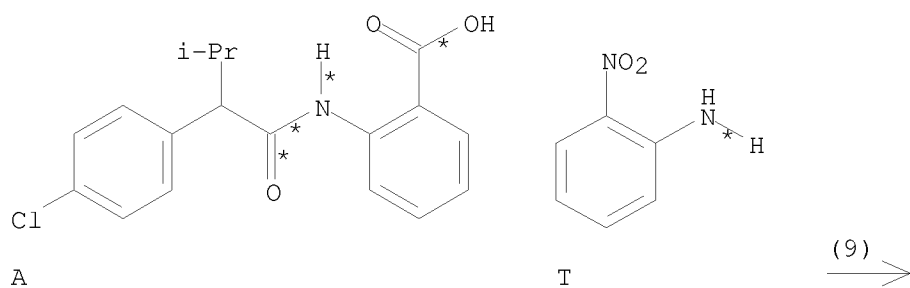
10/ 562,112



S  
YIELD 70%

RX(8)        RCT    A 851191-19-0, R 106-40-1  
              RGT    D 110-86-1 Pyridine  
              PRO    S 851191-10-1  
              SOL    64-17-5 EtOH  
              CON    4 hours, reflux  
              NTE    chemoselective

RX(9) OF 33        ...A + T ==> U



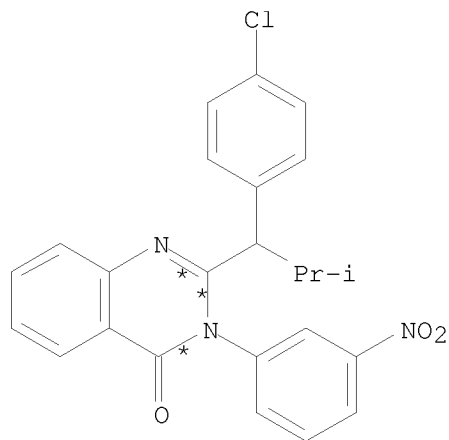
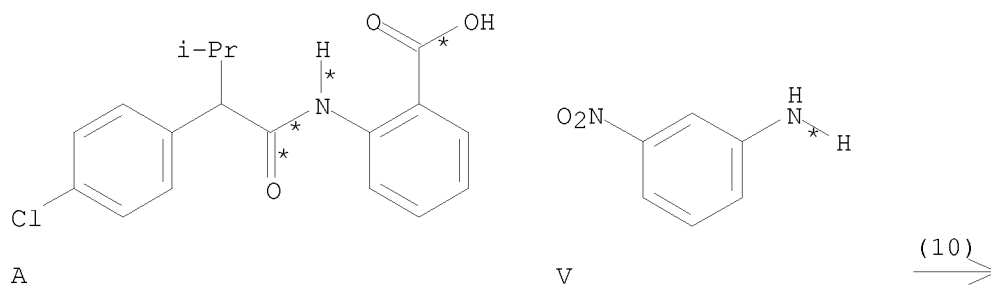
U  
YIELD 64%

RX(9)        RCT    A 851191-19-0, T 88-74-4

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RGT D 110-86-1 Pyridine  
PRO U 851191-11-2  
SOL 64-17-5 EtOH  
CON 4 hours, reflux  
NTE chemoselective

RX(10) OF 33 ...A + V ==> W

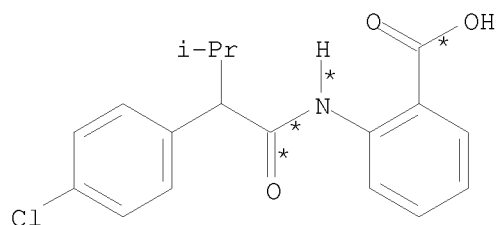


W  
YIELD 76%

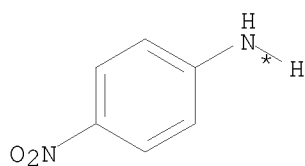
RX(10) RCT A 851191-19-0, V 99-09-2  
RGT D 110-86-1 Pyridine  
PRO W 851191-12-3  
SOL 64-17-5 EtOH  
CON 4 hours, reflux  
NTE chemoselective

RX(11) OF 33 ...A + X ==> Y

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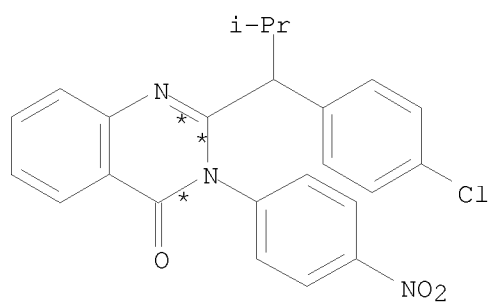


A



X

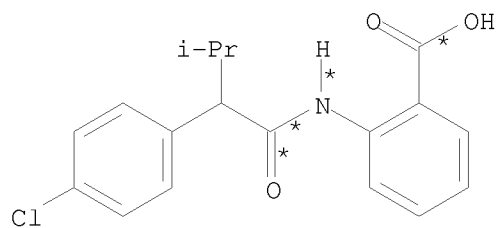
(11)  
→



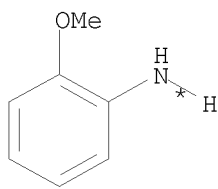
Y  
YIELD 72%

RX(11)      RCT    A 851191-19-0, X 100-01-6  
               RGT    D 110-86-1 Pyridine  
               PRO    Y 851191-13-4  
               SOL    64-17-5 EtOH  
               CON    4 hours, reflux  
               NTE    chemoselective

RX(12) OF 33      ...A + Z ==> AA



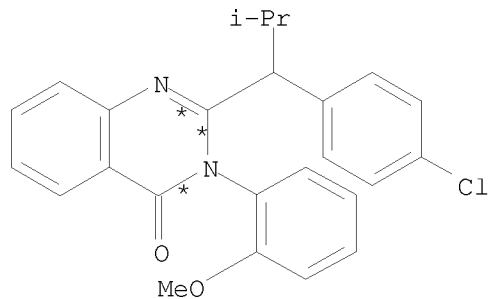
A



Z

(12)  
→

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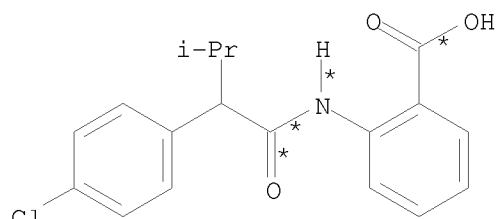


AA

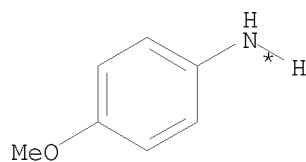
YIELD 80%

RX(12)      RCT    A 851191-19-0, Z 90-04-0  
              RGT    D 110-86-1 Pyridine  
              PRO    AA 851191-14-5  
              SOL    64-17-5 EtOH  
              CON    4 hours, reflux  
              NTE    chemoselective

RX(13) OF 33      ...A + AB ==> AC

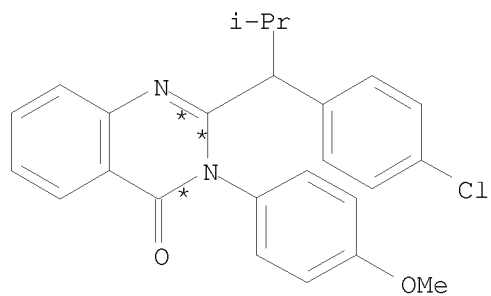


A



AB

(13)  
→



AC

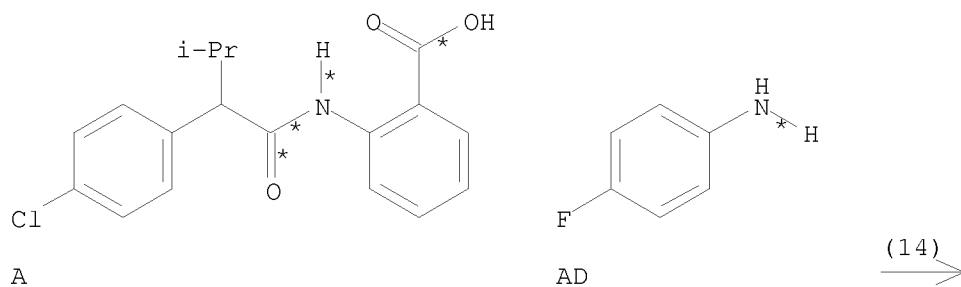
YIELD 78%

RX(13)      RCT    A 851191-19-0, AB 104-94-9  
              RGT    D 110-86-1 Pyridine

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PRO AC 851191-15-6  
SOL 64-17-5 EtOH  
CON 4 hours, reflux  
NTE chemoselective

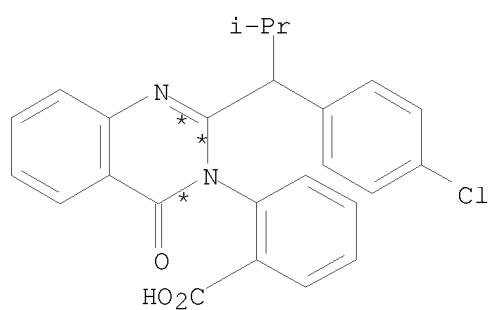
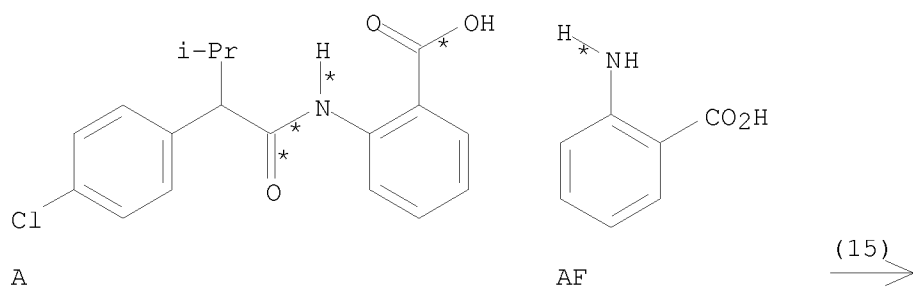
RX(14) OF 33 ...A + AD ==> AE



AE  
YIELD 65%

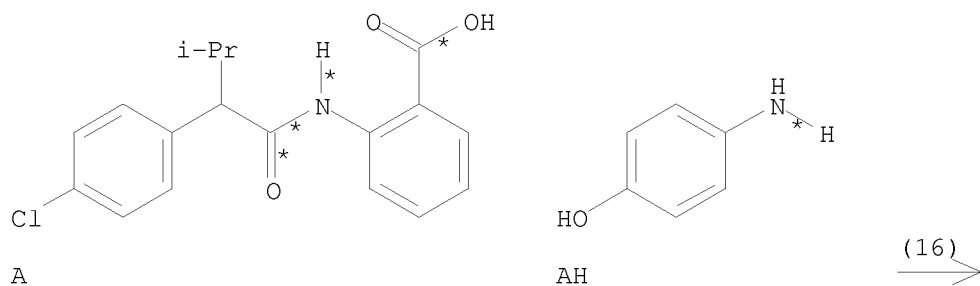
RX(14) RCT A 851191-19-0, AD 371-40-4  
RGT D 110-86-1 Pyridine  
PRO AE 851191-16-7  
SOL 64-17-5 EtOH  
CON 4 hours, reflux  
NTE chemoselective

RX(15) OF 33 ...A + AF ==> AG

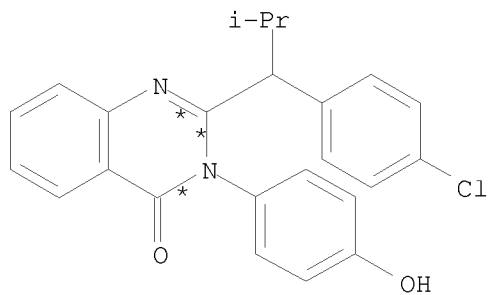


RX(15)     RCT    A 851191-19-0, AF 118-92-3  
              RGT    D 110-86-1 Pyridine  
              PRO    AG 851191-17-8  
              SOL    64-17-5 EtOH  
              CON    4 hours, reflux  
              NTE    chemoselective

RX(16) OF 33     ...A + AH ==> AI



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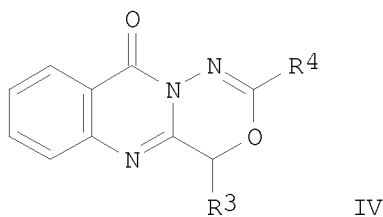
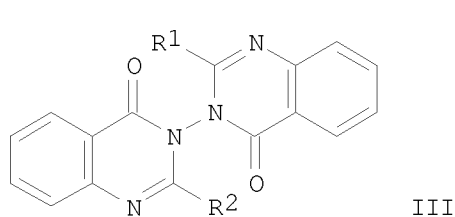
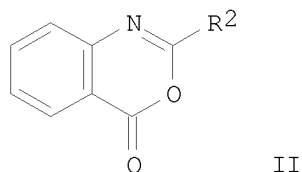
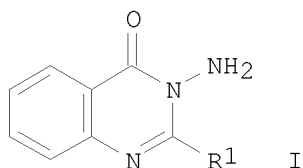
AI  
YIELD 50%

RX(16)	RCT	A 851191-19-0, AH 123-30-8
	RGT	D 110-86-1 Pyridine
	PRO	AI 851191-18-9
	SOL	64-17-5 EtOH
	CON	4 hours, reflux
	NTE	chemoselective

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

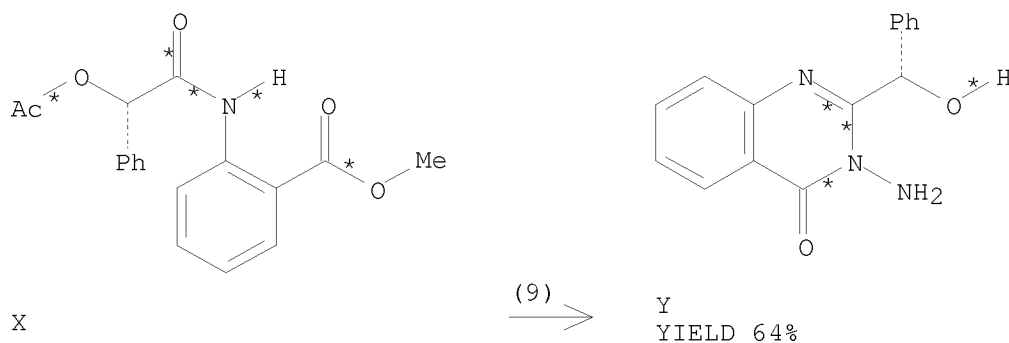
L3 ANSWER 53 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 142:430245 CASREACT  
TITLE: Synthesis of unsymmetrical  
3,3'-biquinazoline-2,2'-diones by condensation of  
3-aminoquinazolinones with benzoxazinones; fortuitous  
discovery, and further syntheses of  
4-H-3-oxa-1,9a,10-triazaanthracen-9-ones  
AUTHOR(S): Coogan, Michael P.; Ooi, Li-ling; Pertusati, Fabrizio  
CORPORATE SOURCE: Department of Chemistry, Cardiff University, Cardiff,  
CF10 3TB, UK  
SOURCE: Organic & Biomolecular Chemistry (2005), 3(6),  
1134-1139  
CODEN: OBCRAK; ISSN: 1477-0520  
PUBLISHER: Royal Society of Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI





AB Condensation of 2-alkyl- or 2-aryl-3-aminoquinazolin-4-ones I ( $R_1 = \text{EtS}, \text{Me}_3\text{C}, \text{EtO}_2\text{C}, \text{Ph}, \text{PhCH}:\text{CHCH}_2\text{CHMe}$ ) with benz[1,3]oxazin-4-ones II ( $R_2 = \text{H}, \text{Me}, \text{Et}$ ) gives the unsym. 2,2'-disubstituted 3,3'-biquinazoline-4,4'-diones III. The reaction is tolerant to a range of heteroatom and unsatd. functionality in the quinazolinone 2-position. However, treatment of 3-amino-2-hydroxymethyl-3H-quinazolin-4-ones I ( $R_1 = \text{R}_3\text{CHOH}; \text{R}_3 = \text{H}, \text{Me}_2\text{CH}, \text{Ph}$ ) with benz[1,3]oxazinone II ( $R_2 = \text{H}$ ) at high temps. gave 4H-3-oxa-1,9a,10-triazaanthracen-9-ones IV, an unreported fused heterocyclic system, a more direct synthesis of which by replacement of benzoxazinones with orthoesters  $\text{R}_4\text{C}(\text{OEt})_3$  ( $\text{R}_4 = \text{H}, \text{Me}, \text{Et}, \text{Ph}$ ) is presented.

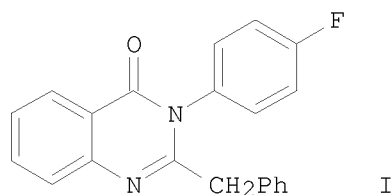
RX(9) OF 21      ...X ==> Y...



RX(9)      RCT   X 850870-21-2  
              RGT   Z 302-01-2 N<sub>2</sub>H<sub>4</sub>  
              PRO   Y 850870-20-1  
              SOL   64-17-5 EtOH  
              CON   5 hours, reflux

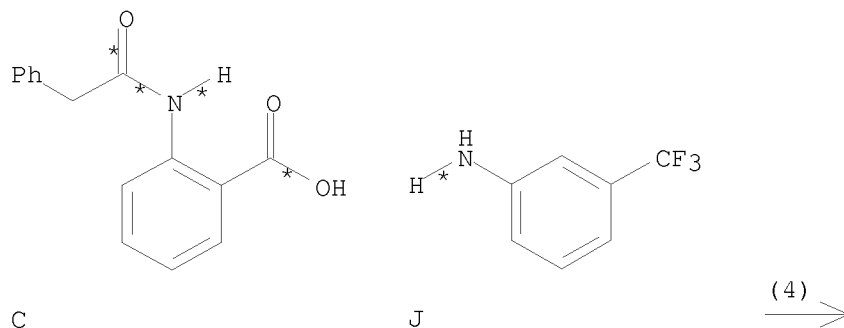
REFERENCE COUNT:      19      THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 54 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 142:316783 CASREACT  
 TITLE: Green chemical multi-component one-pot synthesis of  
 fluorinated 2,3-disubstituted quinazolin-4(3H)-ones  
 under solvent-free conditions and their anti-fungal  
 activity  
 AUTHOR(S): Dandia, Anshu; Singh, Ruby; Sarawgi, Pritima  
 CORPORATE SOURCE: Department of Chemistry, University of Rajasthan,  
 Jaipur, 302004, India  
 SOURCE: Journal of Fluorine Chemistry (2004), 125(12),  
 1835-1840  
 CODEN: JFLCAR; ISSN: 0022-1139  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

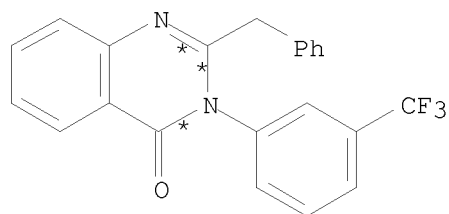


AB A rapid one-pot solvent-free procedure has been developed for the  
 synthesis of fluorinated 2,3-disubstituted quinazolin-4(3H)-ones, e.g., I,  
 by neat three-component cyclocondensation of anthranilic acid, Ph acetyl  
 chloride and substituted anilines under microwave irradiation The exptl.  
 methodol. and microwave conditions described here are well established,  
 allowing significant rate enhancement and good yields compared to  
 conventional reaction conditions. The reaction is generalized for ortho-,  
 meta-, and para-substituted anilines to give quinazolin-4(3H)-ones.  
 Synthesized compds. have been screened for their antifungal activity.

RX(4) OF 19 ...C + J ==> K



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K  
YIELD 88%

RX(4) RCT C 28565-98-2

STAGE(1)

RGT F 292600-93-2 KSF (catalyst)

SOL 108-24-7 Ac2O

CON 3 minutes, 141 deg C

STAGE(2)

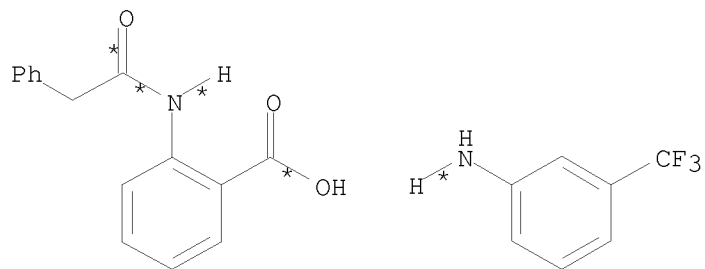
RCT J 98-16-8

CON 7 minutes, 141 deg C

PRO K 848085-19-8

NTE microwave irradiation

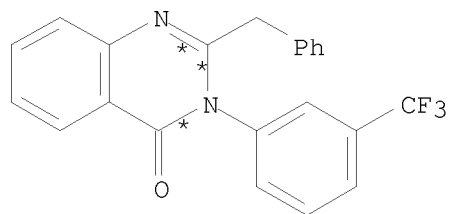
RX(5) OF 19 C + J ==> K



C

J

(5) ➞



K  
YIELD 82%

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RX(5) RCT C 28565-98-2

STAGE(1)

RGT L 1344-28-1 Al2O3

SOL 108-24-7 Ac2O

CON 3 minutes, 132 deg C

STAGE(2)

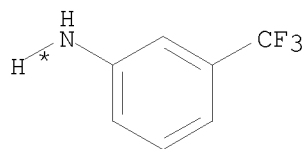
RCT J 98-16-8

CON 10 minutes, 132 deg C

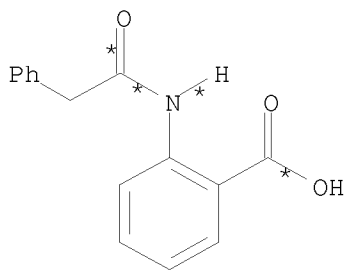
PRO K 848085-19-8

NTE microwave irradiation

RX(7) OF 19 J + C ==> K

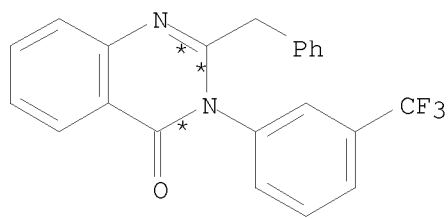


J



C

(7)  $\longrightarrow$



K

YIELD 91%

RX(7) RCT J 98-16-8, C 28565-98-2

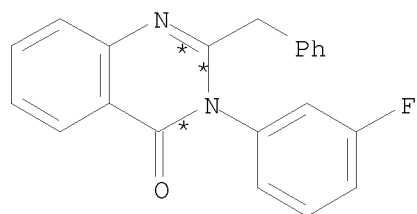
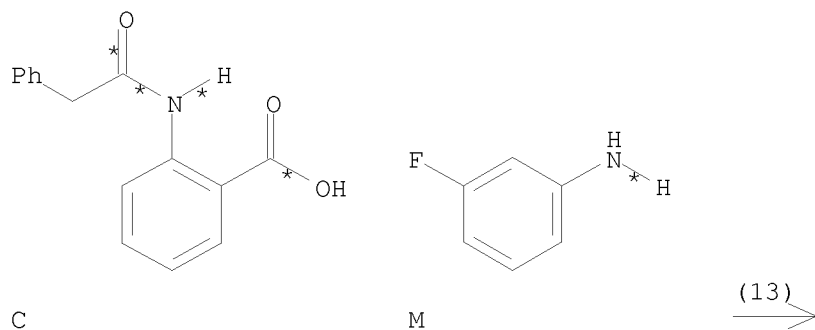
PRO K 848085-19-8

CON 4 minutes, 164 deg C

NTE microwave irradiation

RX(13) OF 19 ...C + M ==> N

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N  
YIELD 82%

RX(13) RCT C 28565-98-2

STAGE(1)

RGT F 292600-93-2 KSF (catalyst)

SOL 108-24-7 Ac2O

CON 3 minutes, 142 deg C

STAGE(2)

RCT M 372-19-0

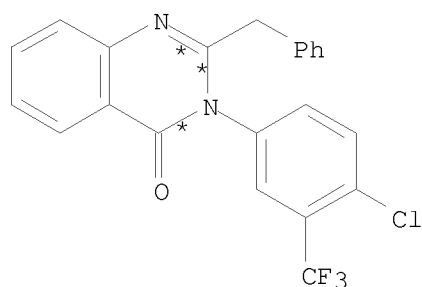
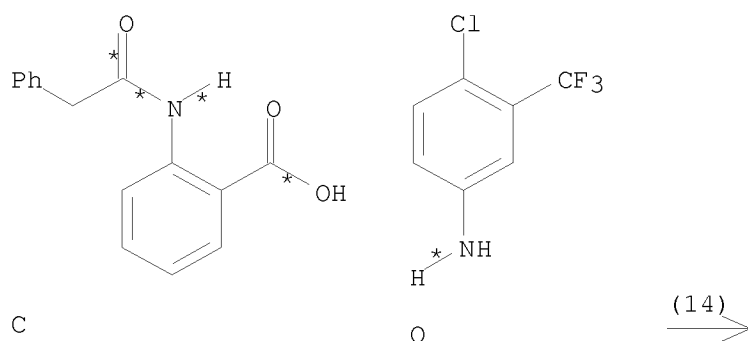
CON 6 minutes, 142 deg C

PRO N 848085-20-1

NTE microwave irradiation

RX(14) OF 19 ...C + O ==> P

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P  
YIELD 81%

RX(14) RCT C 28565-98-2

STAGE(1)

RGT F 292600-93-2 KSF (catalyst)  
SOL 108-24-7 Ac2O  
CON 3 minutes, 137 deg C

STAGE(2)

RCT O 320-51-4  
CON 7 minutes, 137 deg C

PRO P 848085-21-2

NTE microwave irradiation

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 55 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 142:316496 CASREACT

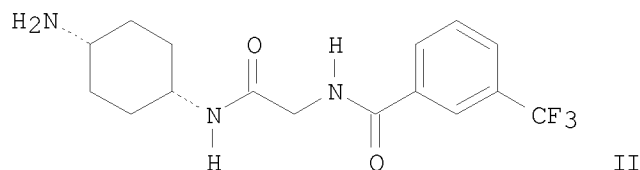
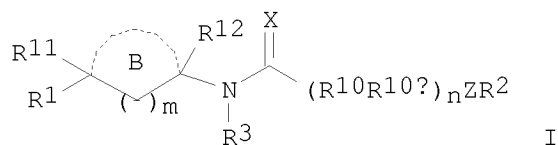
TITLE: Preparation of substituted cycloalkylamine derivatives as modulators of chemokine receptor activity

INVENTOR(S): Carter, Percy H.; Cherney, Robert J.; Batt, Douglas G.; Brown, Gregory D.; Duncia, John V.; Gardner, Daniel S.; Yang, Michael G.

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA  
 SOURCE: PCT Int. Appl., 440 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005020899	A2	20050310	WO 2004-US27195	20040820
WO 2005020899	A3	20050630		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 20050054626	A1	20050310	US 2004-923538	20040819
US 7378409	B2	20080527		
EP 1656138	A2	20060517	EP 2004-781805	20040820
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR			
JP 2007502842	T	20070215	JP 2006-524091	20040820
NO 2006000719	A	20060427	NO 2006-719	20060214
PRIORITY APPLN. INFO.:			US 2003-496974P	20030821
			US 2004-923538	20040819
			WO 2004-US27195	20040820

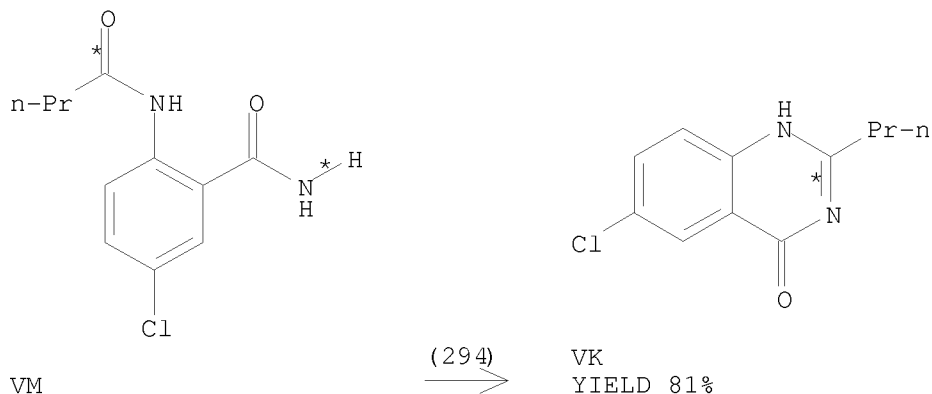
OTHER SOURCE(S): MARPAT 142:316496  
 GI



AB Title compds. I [Ring B = saturated or partially unsatd., (un)substituted cycloalkyl or heterocycle; X = O or S; Z = CO, CONR8, NR8, NR8CO, etc.; R1 = H, (un)substituted-alkyl, -alkenyl, -aryl, etc.; R2 = (un)substituted aryl or heteroaryl; R3 = H, Me, or Et; R8 = H, alkyl, or cycloalkyl; R10 and R10a independently = H or (un)substituted alkyl; R11 = H, alkyl, etc.;

R12 = H, alkyl, (un)substituted carbocycle; m = 0-1; n = 1 or 2], or pharmaceutically acceptable salt forms thereof, are prepared and disclosed as modulators of chemokine receptor activity. Thus, e.g., II was prepared by amidation of trans-4-aminocyclohexanol hydrochloride with (3-trifluoromethylbenzoylamino)acetic acid followed by mesylation, substitution with sodium azide and subsequent reduction. I were deemed active (IC<sub>50</sub> value of 20  $\mu$ M or less) in antagonism of MCP-1 binding to human peripheral blood mononuclear cells. As modulators of MCP-1, I should prove useful for the prevention of asthma, multiple sclerosis, atherosclerosis, and rheumatoid arthritis.

RX(294) OF 1874 ...VM ==> VK...



RX(294) RCT VM 746671-46-5

STAGE(1)

RGT AU 1310-73-2 NaOH  
SOL 7732-18-5 Water, 64-17-5 EtOH  
CON 15 minutes, room temperature

STAGE(2)

RGT G 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, pH 2

PRO VK 69729-73-3

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 56 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 142:240392 CASREACT

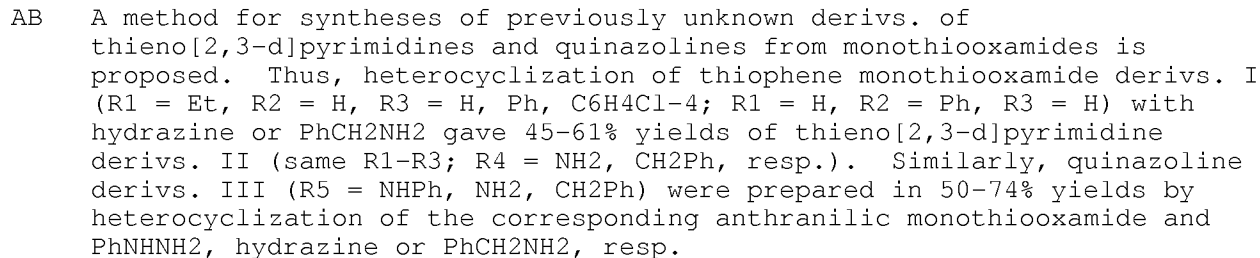
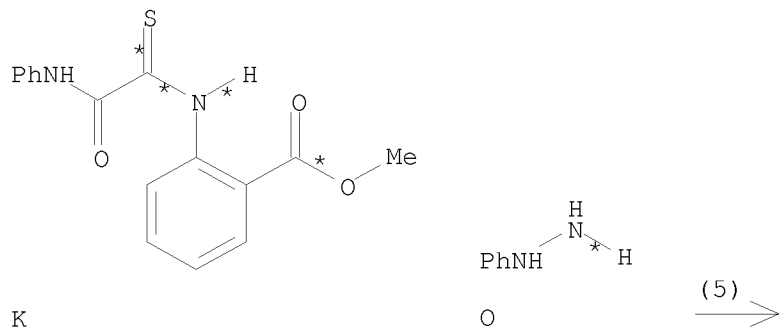
TITLE: Synthesis of thieno[2,3-d]pyrimidine and quinazoline derivatives from monothiooxamides

AUTHOR(S): Zavarzin, I. V.; Smirnova, N. G.; Chernoburova, E. I.; Yarovenko, V. N.; Krayushkin, M. M.

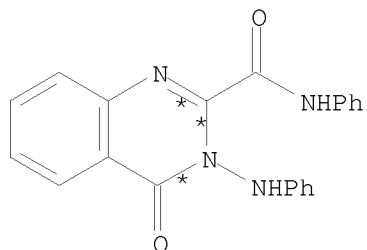
CORPORATE SOURCE: N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, 119991, Russia

SOURCE: Russian Chemical Bulletin (Translation of Izvestiya



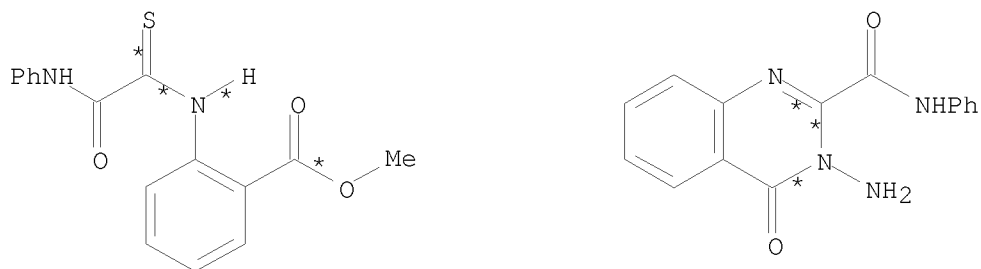

$$RX(5) \text{ OF } 31 \dots K + 0 \implies P$$


10/ 562,112



P  
YIELD 61%

RX(5)	RCT	K 845298-11-5, O 100-63-0
	PRO	P 845298-12-6
	SOL	64-17-5 EtOH
	CON	5 days, reflux

$$RX(6) \text{ OF } 31 \dots K \implies Q$$


K

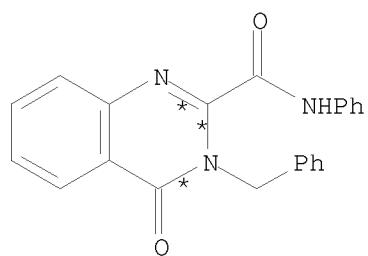
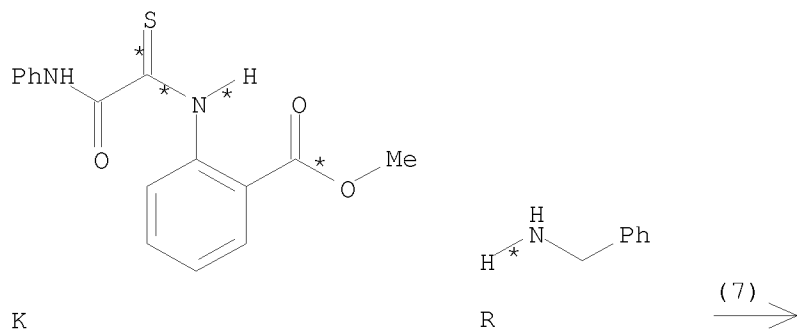
(6) 

Q  
YIELD 50%

RX (6)	RCT	K 845298-11-5
	RGT	C 302-01-2 N2H4
	PRO	Q 845298-13-7
	SOL	64-17-5 EtOH
	CON	3 hours, reflux

$$RX(7) \text{ OF } 31 \quad \dots K \quad + \quad R \quad ==> \quad S$$

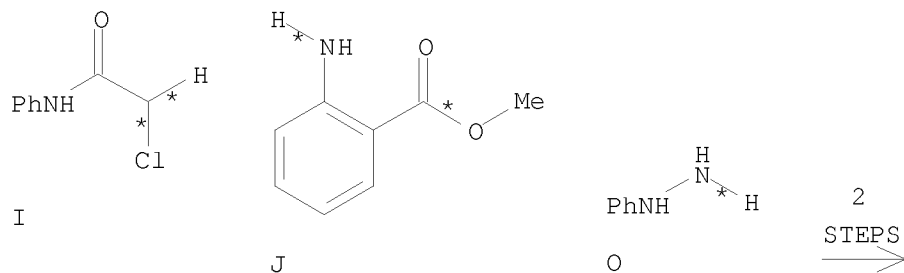
10/ 562,112



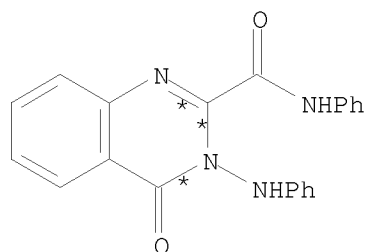
YIELD 75%

RX(7) RCT K 845298-11-5, R 100-46-9  
 PRO S 845298-14-8  
 SOL 100-46-9 PhCH<sub>2</sub>NH<sub>2</sub>  
 CON 20 minutes, reflux

RX(20) OF 31 COMPOSED OF RX(4), RX(5)  
 RX(20) I + J + O ==> P



10/ 562,112

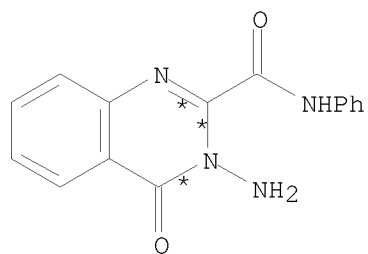
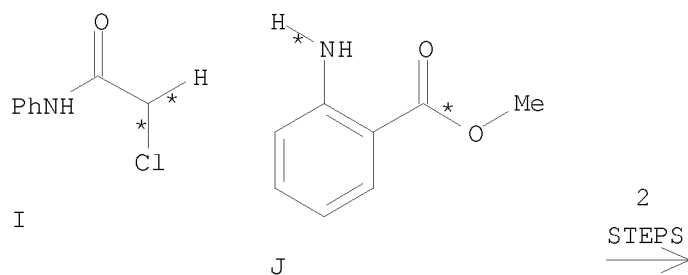


P  
YIELD 61%

RX(4)      RCT    I 587-65-5, J 134-20-3  
             RGT    L 7704-34-9 S, M 121-44-8 Et3N  
             PRO    K 845298-11-5  
             SOL    68-12-2 DMF  
             NTE    conditions not stated

RX(5)      RCT    K 845298-11-5, O 100-63-0  
             PRO    P 845298-12-6  
             SOL    64-17-5 EtOH  
             CON    5 days, reflux

RX(21) OF 31 COMPOSED OF RX(4), RX(6)  
RX(21)      I    +    J    ==>    Q



Q  
YIELD 50%

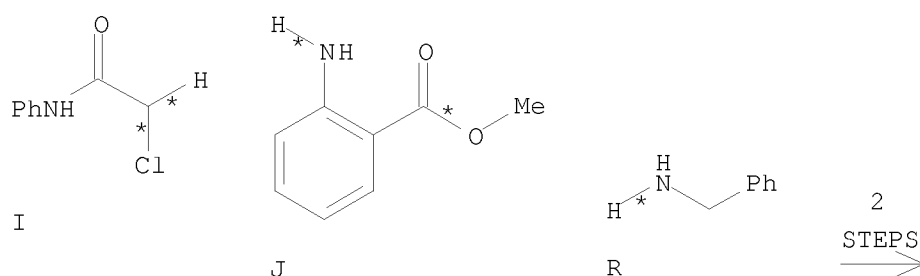
RX(4)      RCT    I 587-65-5, J 134-20-3

10/ 562,112

RGT L 7704-34-9 S, M 121-44-8 Et3N  
PRO K 845298-11-5  
SOL 68-12-2 DMF  
NTE conditions not stated

RX(6) RCT K 845298-11-5  
RGT C 302-01-2 N2H4  
PRO Q 845298-13-7  
SOL 64-17-5 EtOH  
CON 3 hours, reflux

RX(22) OF 31 COMPOSED OF RX(4), RX(7)  
RX(22) I + J + R ==> S



S  
YIELD 75%

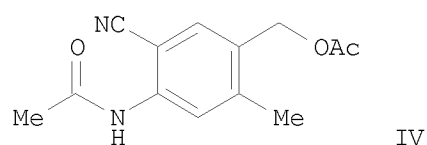
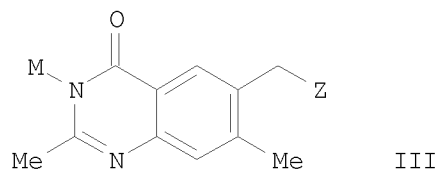
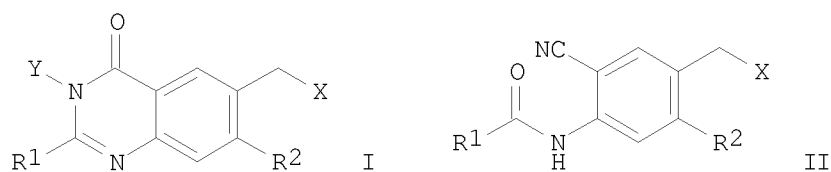
RX(4) RCT I 587-65-5, J 134-20-3  
RGT L 7704-34-9 S, M 121-44-8 Et3N  
PRO K 845298-11-5  
SOL 68-12-2 DMF  
NTE conditions not stated

RX(7) RCT K 845298-11-5, R 100-46-9  
PRO S 845298-14-8  
SOL 100-46-9 PhCH2NH2  
CON 20 minutes, reflux

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

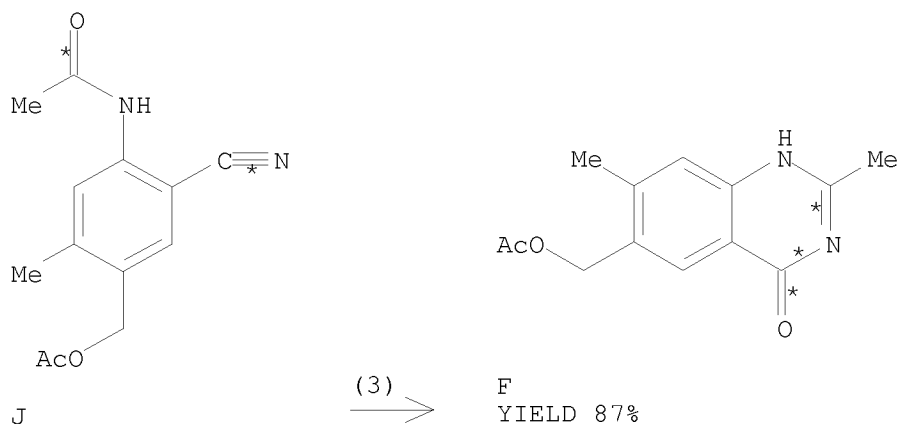
L3 ANSWER 57 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 142:198095 CASREACT  
 TITLE: A preparation of quinazolin-4-ones via cyclization of  
 N-(cyanophenyl)acetamide derivatives  
 INVENTOR(S): Godfrey, Andrew Aydon  
 PATENT ASSIGNEE(S): BTG International Limited, UK  
 SOURCE: PCT Int. Appl., 29 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005012260	A2	20050210	WO 2004-GB3141	20040720
WO 2005012260	A3	20050407		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2004261453	A1	20050210	AU 2004-261453	20040720
CA 2531750	A1	20050210	CA 2004-2531750	20040720
EP 1675831	A2	20060705	EP 2004-743476	20040720
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK			
JP 2007500175	T	20070111	JP 2006-521644	20040720
US 20060189804	A1	20060824	US 2005-562112	20051223
IN 2006DN00057	A	20070824	IN 2006-DN57	20060103
MX 2006000883	A	20060419	MX 2006-883	20060123
KR 2006056962	A	20060525	KR 2006-701909	20060127
PRIORITY APPLN. INFO.:			GB 2003-17631	20030728
			WO 2004-GB3141	20040720
OTHER SOURCE(S):	MARPAT 142:198095			
GI				



AB The invention relates to a preparation of quinazolin-4-one derivs. of formula I [wherein: R1 and R2 are independently H or Me; Y is a protecting group; X is a leaving group], useful as intermediates in preparation of antitumor agents. The invention compds. I were prepared via cyclization of amides of formula II. For instance, quinazolin-4-one derivative III•HBr (Z = Br, M = H) was prepared via intramol. cyclization of N-(cyanophenyl)acetamide derivative IV, N-protection of the obtained quinazoline derivative III (Z = OAc; M = H) by chloromethyl pivalate, and subsequent bromination (yields: cyclization - 87%, bromination - 89%).

RX(3) OF 45      ...J ==> F...

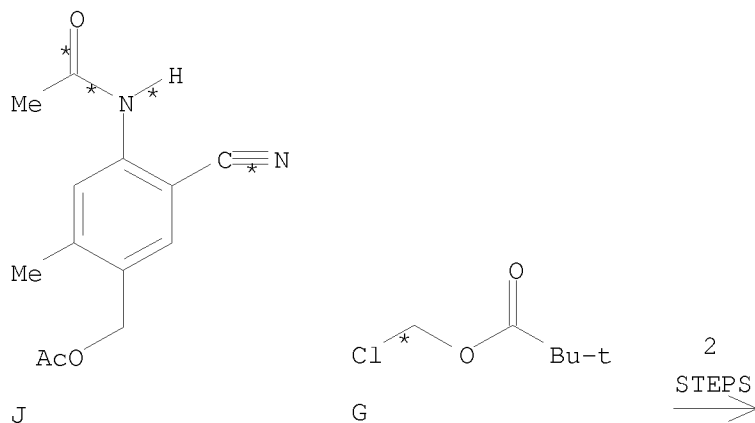


RX(3)      RCT   J 838858-87-0  
             RGT   K 7647-01-0 HCl

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PRO F 838858-86-9  
SOL 67-63-0 Me2CHOH  
CON SUBSTAGE(1) 60 minutes  
SUBSTAGE(2) 30 deg C  
NTE HCl gas used

RX(12) OF 45 COMPOSED OF RX(3), RX(2)  
RX(12) J + G ==> A



A  
YIELD 62%

RX(3) RCT J 838858-87-0  
RGT K 7647-01-0 HCl  
PRO F 838858-86-9  
SOL 67-63-0 Me2CHOH  
CON SUBSTAGE(1) 60 minutes  
SUBSTAGE(2) 30 deg C  
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)  
RGT H 584-08-7 K2CO3  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)  
RCT G 18997-19-8



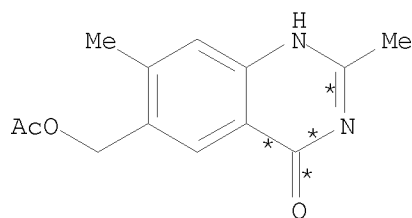
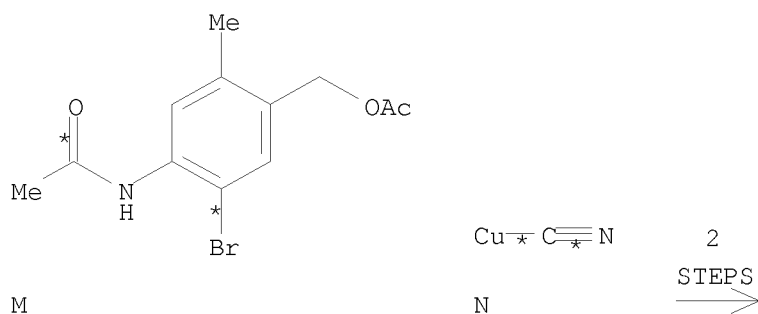
10/ 562,112

CON SUBSTAGE(1) 2.5 hours, 50 deg C  
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(13) OF 45 COMPOSED OF RX(4), RX(3)

RX(13) M + N ==> F



F  
YIELD 87%

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0

NTE inert, incremental addition of reagent in second stage

RX(3)

RCT J 838858-87-0

RGT K 7647-01-0 HCl

PRO F 838858-86-9

SOL 67-63-0 Me2CHOH

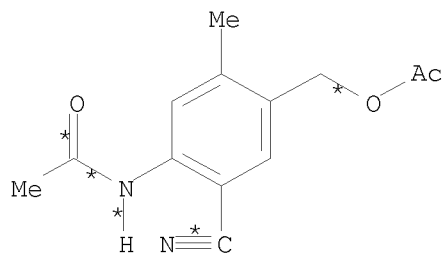
CON SUBSTAGE(1) 60 minutes

SUBSTAGE(2) 30 deg C

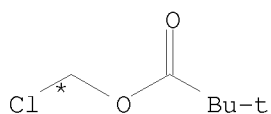
NTE HCl gas used

10/ 562,112

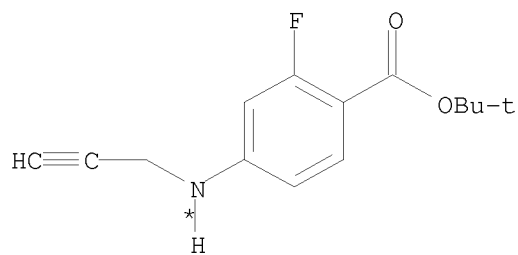
RX(21) OF 45 COMPOSED OF RX(3), RX(2), RX(1), RX(9)  
RX(21) J + G + AI ==> AG



J

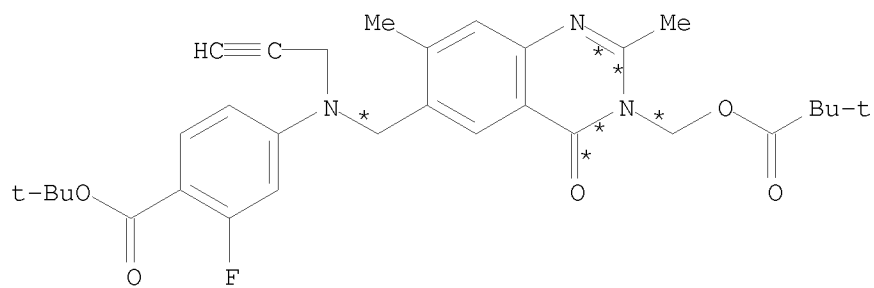


G



AI

4  
STEPS  
➤



AG

YIELD 80%

RX(3) RCT J 838858-87-0  
RGT K 7647-01-0 HCl  
PRO F 838858-86-9  
SOL 67-63-0 Me2CHOH  
CON SUBSTAGE(1) 60 minutes  
SUBSTAGE(2) 30 deg C  
NTE HCl gas used

RX(2) RCT F 838858-86-9

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STAGE(1)  
RGT H 584-08-7 K2CO3  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)  
RCT G 18997-19-8  
CON SUBSTAGE(1) 2.5 hours, 50 deg C  
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) 2 hours, 60 deg C  
SUBSTAGE(2) 3 hours, 60 deg C  
SUBSTAGE(3) 60 deg C -> 16 deg C  
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

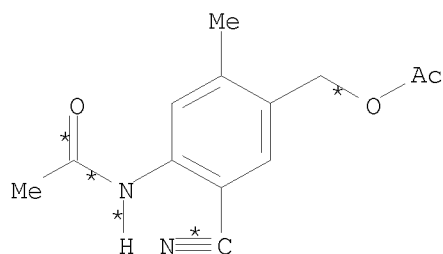
STAGE(1)  
RGT AJ 144-55-8 NaHCO3  
SOL 7732-18-5 Water, 108-88-3 PhMe  
CON SUBSTAGE(1) 30 minutes, 65 deg C  
SUBSTAGE(2) 1 hour

STAGE(2)  
RCT AI 140373-03-1  
RGT AK 108-48-5 2,6-Lutidine  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) 105 deg C  
SUBSTAGE(2) 24 hours, 105 deg C  
SUBSTAGE(3) 105 deg C -> 65 deg C

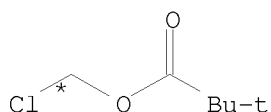
PRO AG 153538-14-8

RX(22) OF 45 COMPOSED OF RX(3), RX(2), RX(1)  
RX(22) J + G ==> B

10/ 562,112

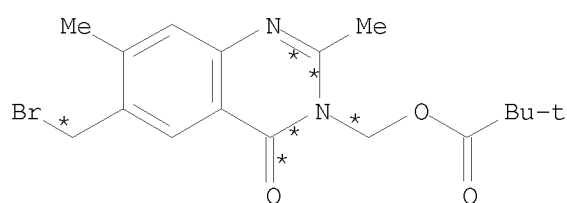


J



G

3  
STEPS  
→



● HBr

B  
YIELD 89%

RX(3) RCT J 838858-87-0  
RGT K 7647-01-0 HCl  
PRO F 838858-86-9  
SOL 67-63-0 Me<sub>2</sub>CHOH  
CON SUBSTAGE(1) 60 minutes  
SUBSTAGE(2) 30 deg C  
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)  
RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)  
RCT G 18997-19-8  
CON SUBSTAGE(1) 2.5 hours, 50 deg C  
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)  
RGT C 10035-10-6 HBr

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SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 60 deg C

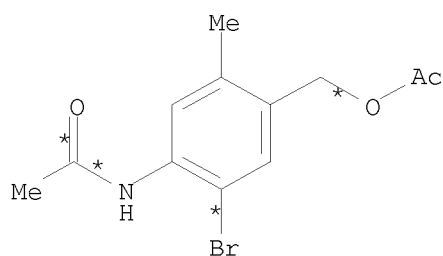
STAGE(2)

RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) 2 hours, 60 deg C  
SUBSTAGE(2) 3 hours, 60 deg C  
SUBSTAGE(3) 60 deg C -> 16 deg C  
SUBSTAGE(4) 18 hours, 16 deg C

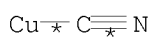
PRO B 838858-84-7

RX(23) OF 45 COMPOSED OF RX(4), RX(3), RX(2), RX(1)

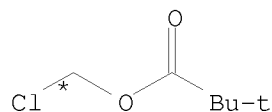
RX(23) M + N + G ==> B



M



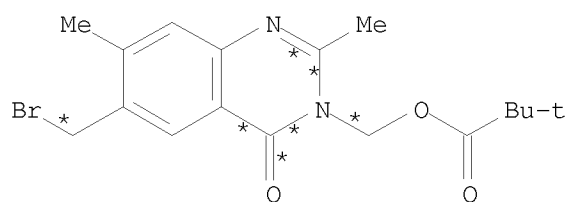
N



G

4

STEPS  
=>



● HBr

B  
YIELD 89%

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF  
CON SUBSTAGE(1) 6 hours, 90 deg C

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SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0

NTE inert, incremental addition of reagent in second stage

RX(3)

RCT J 838858-87-0

RGT K 7647-01-0 HCl

PRO F 838858-86-9

SOL 67-63-0 Me2CHOH

CON SUBSTAGE(1) 60 minutes

SUBSTAGE(2) 30 deg C

NTE HCl gas used

RX(2)

RCT F 838858-86-9

STAGE(1)

RGT H 584-08-7 K2CO3

SOL 67-68-5 DMSO

CON SUBSTAGE(1) 50 deg C

SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)

RCT G 18997-19-8

CON SUBSTAGE(1) 2.5 hours, 50 deg C

SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1)

RCT A 838858-85-8

STAGE(1)

RGT C 10035-10-6 HBr

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)

RGT C 10035-10-6 HBr

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) 2 hours, 60 deg C

SUBSTAGE(2) 3 hours, 60 deg C

SUBSTAGE(3) 60 deg C -> 16 deg C

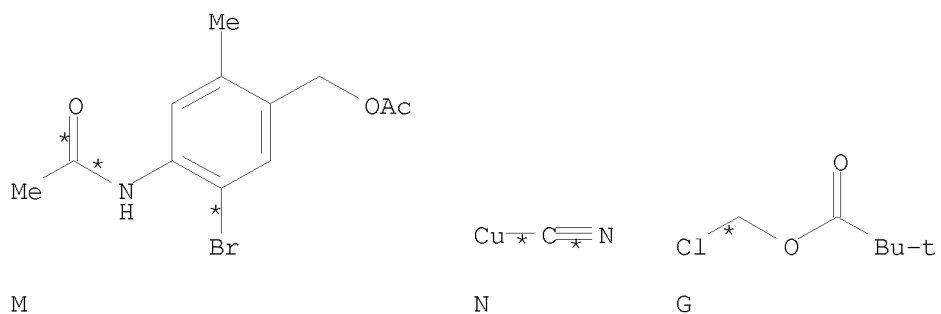
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(24) OF 45 COMPOSED OF RX(4), RX(3), RX(2)

RX(24) M + N + G ==> A

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A  
YIELD 62%

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0

NTE inert, incremental addition of reagent in second stage

RX(3)

RCT J 838858-87-0

RGT K 7647-01-0 HCl

PRO F 838858-86-9

SOL 67-63-0 Me2CHOH

CON SUBSTAGE(1) 60 minutes

SUBSTAGE(2) 30 deg C

NTE HCl gas used

RX(2)

RCT F 838858-86-9

STAGE(1)

RGT H 584-08-7 K2CO3

SOL 67-68-5 DMSO

CON SUBSTAGE(1) 50 deg C

SUBSTAGE(2) 16 hours, 50 deg C

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STAGE(2)

RCT G 18997-19-8

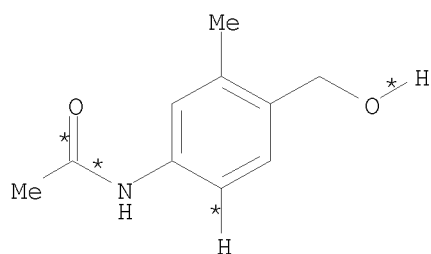
CON SUBSTAGE(1) 2.5 hours, 50 deg C

SUBSTAGE(2) 30 minutes, 50 deg C

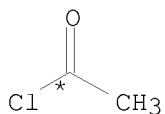
PRO A 838858-85-8

RX(25) OF 45 COMPOSED OF RX(5), RX(4), RX(3), RX(2)

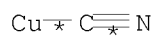
RX(25) Q + R + N + G ==> A



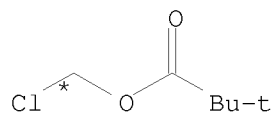
Q



R

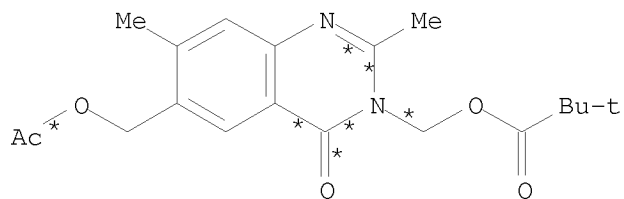


N



G

4  
STEPS  
→



A

YIELD 62%

RX(5) RCT Q 117523-91-8

STAGE(1)

RGT S 121-44-8 Et3N

SOL 141-78-6 AcOEt

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)

RCT R 75-36-5

CON SUBSTAGE(1) 2 hours, 50 deg C



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SUBSTAGE(2) 30 minutes, 50 deg C  
SUBSTAGE(3) 50 deg C -> 20 deg C

STAGE(3)

RGT T 1715-40-8 Bicyclo[2.2.1]hept-2-ene,  
5-(bromomethyl)-1,2,3,4,7,7-hexachloro-  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 60 minutes  
SUBSTAGE(3) 50 deg C -> 20 deg C

PRO M 838858-88-1  
NTE regioselective

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF  
CON SUBSTAGE(1) 6 hours, 90 deg C  
SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn  
CON SUBSTAGE(1) 60 deg C  
SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0  
NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0  
RGT K 7647-01-0 HCl  
PRO F 838858-86-9  
SOL 67-63-0 Me2CHOH  
CON SUBSTAGE(1) 60 minutes  
SUBSTAGE(2) 30 deg C  
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)

RGT H 584-08-7 K2CO3  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 16 hours, 50 deg C

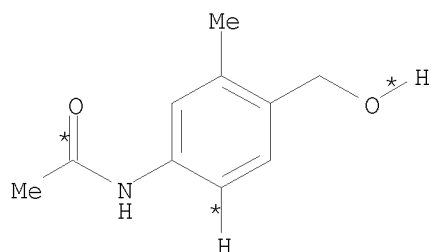
STAGE(2)

RCT G 18997-19-8  
CON SUBSTAGE(1) 2.5 hours, 50 deg C  
SUBSTAGE(2) 30 minutes, 50 deg C

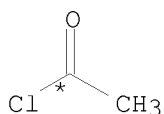
PRO A 838858-85-8

RX(26) OF 45 COMPOSED OF RX(5), RX(4), RX(3)  
RX(26) Q + R + N ==> F

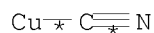
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Q

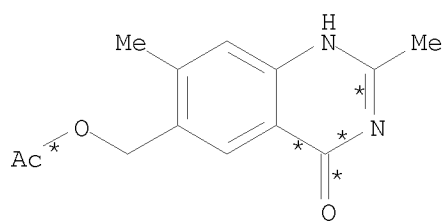


R



N

3  
STEPS  
→



F  
YIELD 87%

RX(5) RCT Q 117523-91-8

STAGE(1)

RGT S 121-44-8 Et3N

SOL 141-78-6 AcOEt

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)

RCT R 75-36-5

CON SUBSTAGE(1) 2 hours, 50 deg C

SUBSTAGE(2) 30 minutes, 50 deg C

SUBSTAGE(3) 50 deg C -> 20 deg C

STAGE(3)

RGT T 1715-40-8 Bicyclo[2.2.1]hept-2-ene,  
5-(bromomethyl)-1,2,3,4,7,7-hexachloro-

SOL 75-05-8 MeCN

CON SUBSTAGE(1) 50 deg C

SUBSTAGE(2) 60 minutes

SUBSTAGE(3) 50 deg C -> 20 deg C

PRO M 838858-88-1

NTE regioselective

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

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SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0

NTE inert, incremental addition of reagent in second stage

RX(3)

RCT J 838858-87-0

RGT K 7647-01-0 HCl

PRO F 838858-86-9

SOL 67-63-0 Me2CHOH

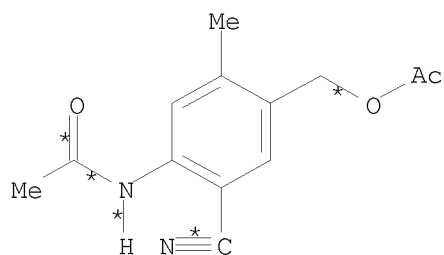
CON SUBSTAGE(1) 60 minutes

SUBSTAGE(2) 30 deg C

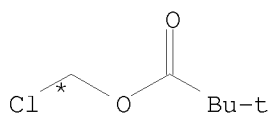
NTE HCl gas used

RX(34) OF 45 COMPOSED OF RX(3), RX(2), RX(1), RX(9), RX(8), RX(7), RX(6)

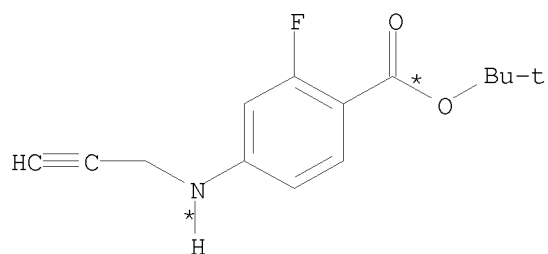
RX(34) J + G + AI + AC ==> X



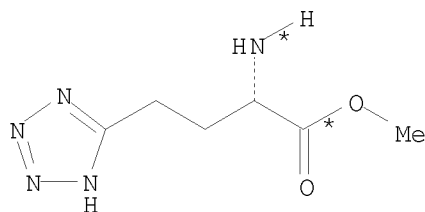
J



G



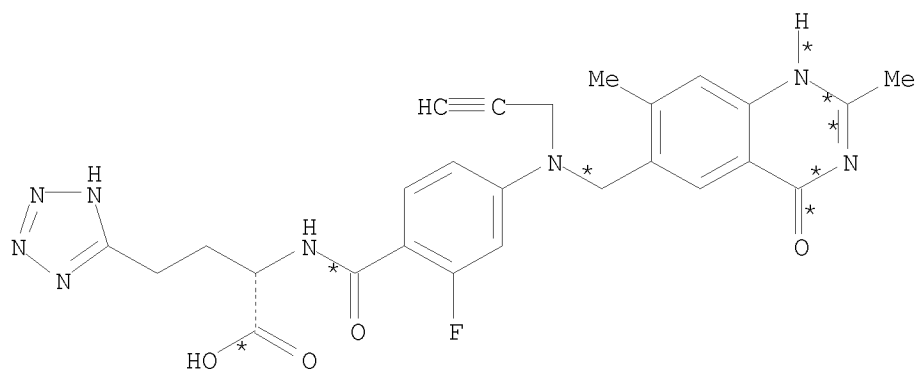
AI



AC

7

STEPS  
→



X  
YIELD 92%

RX(3) RCT J 838858-87-0  
RGT K 7647-01-0 HCl  
PRO F 838858-86-9  
SOL 67-63-0 Me2CHOH  
CON SUBSTAGE(1) 60 minutes  
SUBSTAGE(2) 30 deg C  
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)  
RGT H 584-08-7 K2CO3  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)  
RCT G 18997-19-8  
CON SUBSTAGE(1) 2.5 hours, 50 deg C  
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) 2 hours, 60 deg C  
SUBSTAGE(2) 3 hours, 60 deg C  
SUBSTAGE(3) 60 deg C -> 16 deg C  
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

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RX(9) RCT B 838858-84-7

STAGE(1)

RGT AJ 144-55-8 NaHCO<sub>3</sub>  
SOL 7732-18-5 Water, 108-88-3 PhMe  
CON SUBSTAGE(1) 30 minutes, 65 deg C  
SUBSTAGE(2) 1 hour

STAGE(2)

RCT AI 140373-03-1  
RGT AK 108-48-5 2,6-Lutidine  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) 105 deg C  
SUBSTAGE(2) 24 hours, 105 deg C  
SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

STAGE(1)

RGT AH 64-18-6 HCO<sub>2</sub>H  
SOL 7732-18-5 Water  
CON 5 hours, 40 deg C

STAGE(2)

RGT D 7732-18-5 Water  
CON 3 hours

PRO AB 140373-09-7

RX(7) RCT AB 140373-09-7

STAGE(1)

RGT AD 7719-09-7 SOCl<sub>2</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON SUBSTAGE(1) 30 minutes, 10 deg C  
SUBSTAGE(2) 10 deg C -> 20 deg C

STAGE(2)

RCT AC 127105-49-1  
RGT AE 7087-68-5 EtN(Pr-i)<sub>2</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON SUBSTAGE(1) 3 hours, 10 deg C  
SUBSTAGE(2) 16 hours

STAGE(3)

RGT E 64-19-7 AcOH

PRO W 247904-63-8

NTE inert

RX(6) RCT W 247904-63-8

STAGE(1)

RGT Y 1310-73-2 NaOH  
SOL 7732-18-5 Water, 109-99-9 THF  
CON SUBSTAGE(1) 15 deg C  
SUBSTAGE(2) 15 deg C -> 24 deg C

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SUBSTAGE(3) 19 hours, 24 deg C

STAGE(2)

RGT Z 7631-90-5 NaHSO<sub>3</sub>

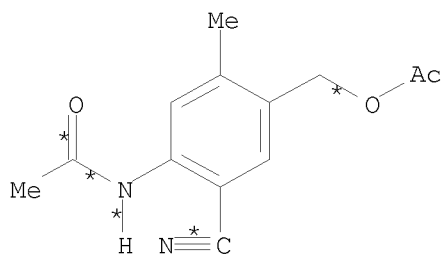
SOL 7732-18-5 Water

CON 40 minutes, 24 deg C

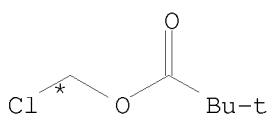
PRO X 153537-73-6

RX(35) OF 45 COMPOSED OF RX(3), RX(2), RX(1), RX(9), RX(8), RX(7)

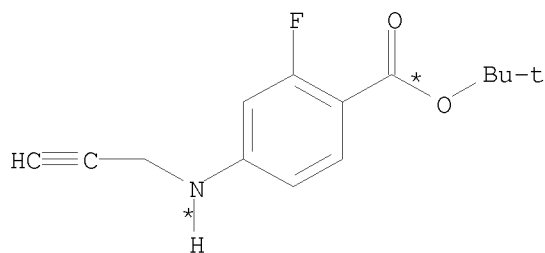
RX(35) J + G + AI + AC ==> W



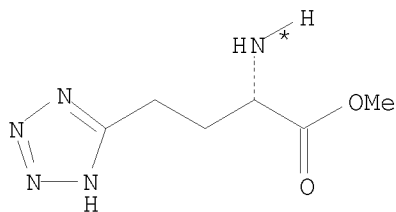
J



G



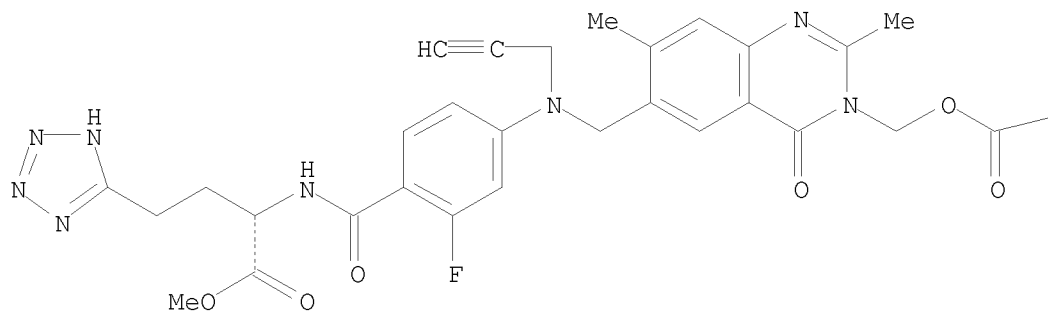
AI



AC

6

STEPS  
→



—Bu-t

W  
YIELD 82%

RX(3) RCT J 838858-87-0  
RGT K 7647-01-0 HCl  
PRO F 838858-86-9  
SOL 67-63-0 Me<sub>2</sub>CHOH  
CON SUBSTAGE(1) 60 minutes  
SUBSTAGE(2) 30 deg C  
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)  
RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)  
RCT G 18997-19-8  
CON SUBSTAGE(1) 2.5 hours, 50 deg C  
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)  
RGT C 10035-10-6 HBr

SOL 7732-18-5 Water, 64-19-7 AcOH  
 CON SUBSTAGE(1) 2 hours, 60 deg C  
 SUBSTAGE(2) 3 hours, 60 deg C  
 SUBSTAGE(3) 60 deg C -> 16 deg C  
 SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)  
 RGT AJ 144-55-8 NaHCO<sub>3</sub>  
 SOL 7732-18-5 Water, 108-88-3 PhMe  
 CON SUBSTAGE(1) 30 minutes, 65 deg C  
 SUBSTAGE(2) 1 hour

STAGE(2)  
 RCT AI 140373-03-1  
 RGT AK 108-48-5 2,6-Lutidine  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) 105 deg C  
 SUBSTAGE(2) 24 hours, 105 deg C  
 SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

STAGE(1)  
 RGT AH 64-18-6 HCO<sub>2</sub>H  
 SOL 7732-18-5 Water  
 CON 5 hours, 40 deg C

STAGE(2)  
 RGT D 7732-18-5 Water  
 CON 3 hours

PRO AB 140373-09-7

RX(7) RCT AB 140373-09-7

STAGE(1)  
 RGT AD 7719-09-7 SOCl<sub>2</sub>  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON SUBSTAGE(1) 30 minutes, 10 deg C  
 SUBSTAGE(2) 10 deg C -> 20 deg C

STAGE(2)  
 RCT AC 127105-49-1  
 RGT AE 7087-68-5 EtN(Pr-i)<sub>2</sub>  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON SUBSTAGE(1) 3 hours, 10 deg C  
 SUBSTAGE(2) 16 hours

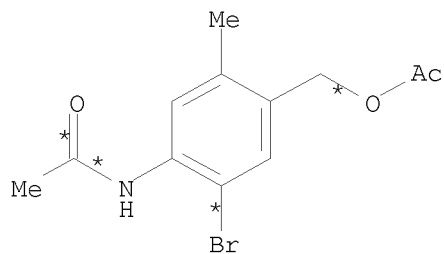
STAGE(3)  
 RGT E 64-19-7 AcOH

PRO W 247904-63-8  
 NTE inert

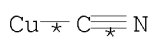


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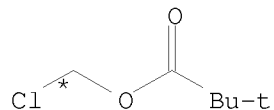
RX(36) OF 45 COMPOSED OF RX(4), RX(3), RX(2), RX(1), RX(9), RX(8), RX(7), RX(6)  
 RX(36) M + N + G + AI + AC ==> X



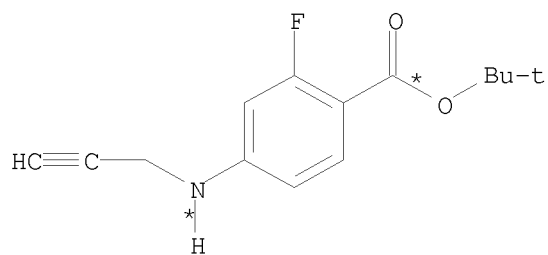
M



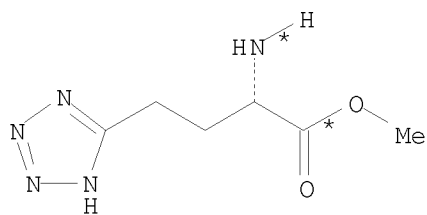
N



G

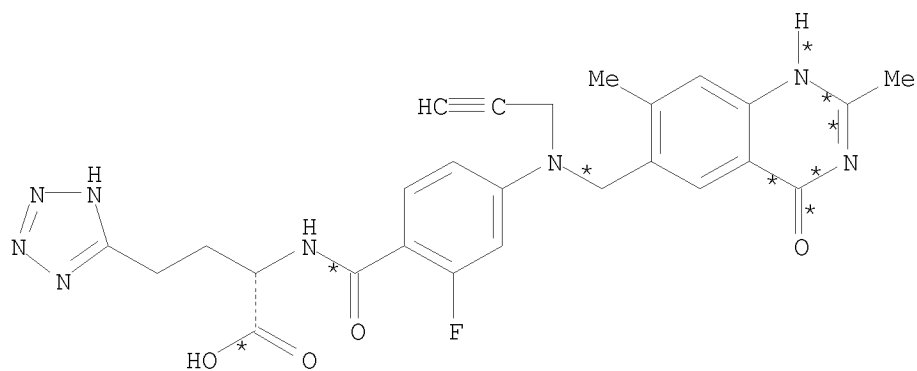


AI



AC

8  
 STEPS  
 →



X  
 YIELD 92%

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 6 hours, 90 deg C  
SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)  
RGT O 7440-66-6 Zn  
CON SUBSTAGE(1) 60 deg C  
SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0  
NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0  
RGT K 7647-01-0 HCl  
PRO F 838858-86-9  
SOL 67-63-0 Me2CHOH  
CON SUBSTAGE(1) 60 minutes  
SUBSTAGE(2) 30 deg C  
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)  
RGT H 584-08-7 K2CO3  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)  
RCT G 18997-19-8  
CON SUBSTAGE(1) 2.5 hours, 50 deg C  
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) 2 hours, 60 deg C  
SUBSTAGE(2) 3 hours, 60 deg C  
SUBSTAGE(3) 60 deg C -> 16 deg C  
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)  
RGT AJ 144-55-8 NaHCO3  
SOL 7732-18-5 Water, 108-88-3 PhMe

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CON SUBSTAGE(1) 30 minutes, 65 deg C  
SUBSTAGE(2) 1 hour

STAGE(2)

RCT AI 140373-03-1  
RGT AK 108-48-5 2,6-Lutidine  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) 105 deg C  
SUBSTAGE(2) 24 hours, 105 deg C  
SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

STAGE(1)

RGT AH 64-18-6 HCO<sub>2</sub>H  
SOL 7732-18-5 Water  
CON 5 hours, 40 deg C

STAGE(2)

RGT D 7732-18-5 Water  
CON 3 hours

PRO AB 140373-09-7

RX(7) RCT AB 140373-09-7

STAGE(1)

RGT AD 7719-09-7 SOCl<sub>2</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON SUBSTAGE(1) 30 minutes, 10 deg C  
SUBSTAGE(2) 10 deg C -> 20 deg C

STAGE(2)

RCT AC 127105-49-1  
RGT AE 7087-68-5 EtN(Pr-i)<sub>2</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON SUBSTAGE(1) 3 hours, 10 deg C  
SUBSTAGE(2) 16 hours

STAGE(3)

RGT E 64-19-7 AcOH

PRO W 247904-63-8

NTE inert

RX(6) RCT W 247904-63-8

STAGE(1)

RGT Y 1310-73-2 NaOH  
SOL 7732-18-5 Water, 109-99-9 THF  
CON SUBSTAGE(1) 15 deg C  
SUBSTAGE(2) 15 deg C -> 24 deg C  
SUBSTAGE(3) 19 hours, 24 deg C

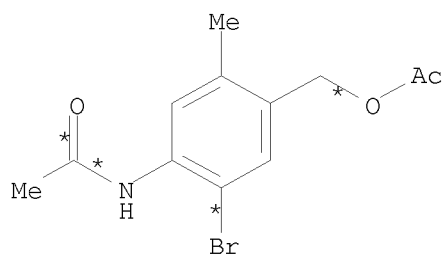
STAGE(2)

RGT Z 7631-90-5 NaHSO<sub>3</sub>  
SOL 7732-18-5 Water  
CON 40 minutes, 24 deg C

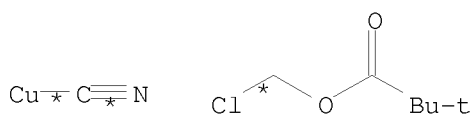
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PRO X 153537-73-6

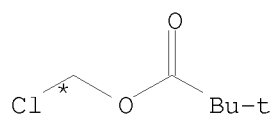
RX(37) OF 45 COMPOSED OF RX(4), RX(3), RX(2), RX(1), RX(9), RX(8), RX(7)  
 RX(37) M + N + G + AI + AC ==> W



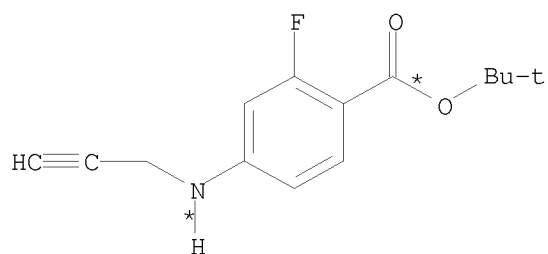
M



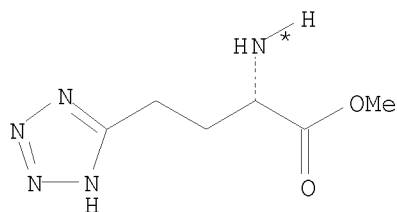
N



G



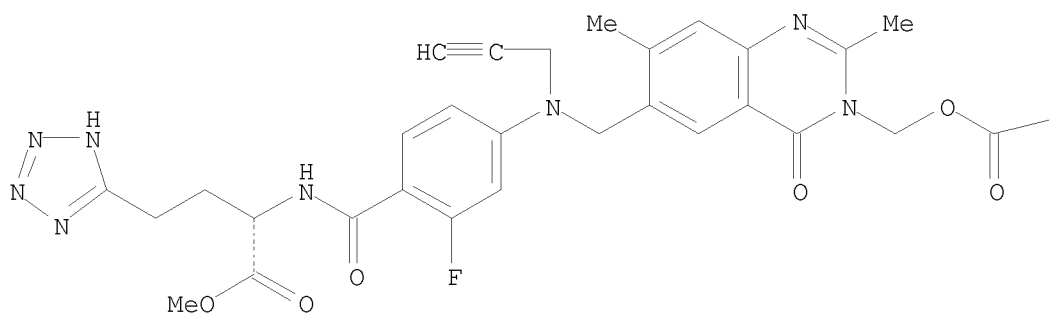
AI



AC

7  
 STEPS  
 →

PAGE 1-A



—Bu-t

W  
YIELD 82%

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0

NTE inert, incremental addition of reagent in second stage

RX(3)

RCT J 838858-87-0

RGT K 7647-01-0 HCl

PRO F 838858-86-9

SOL 67-63-0 Me2CHOH

CON SUBSTAGE(1) 60 minutes

SUBSTAGE(2) 30 deg C

NTE HCl gas used

RX(2)

RCT F 838858-86-9

STAGE(1)

RGT H 584-08-7 K2CO3

SOL 67-68-5 DMSO

CON SUBSTAGE(1) 50 deg C

SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)

RCT G 18997-19-8

CON SUBSTAGE(1) 2.5 hours, 50 deg C

SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1)

RCT A 838858-85-8

STAGE(1)

RGT C 10035-10-6 HBr

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)

RGT C 10035-10-6 HBr

SOL 7732-18-5 Water, 64-19-7 AcOH  
 CON SUBSTAGE(1) 2 hours, 60 deg C  
 SUBSTAGE(2) 3 hours, 60 deg C  
 SUBSTAGE(3) 60 deg C -> 16 deg C  
 SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)  
 RGT AJ 144-55-8 NaHCO<sub>3</sub>  
 SOL 7732-18-5 Water, 108-88-3 PhMe  
 CON SUBSTAGE(1) 30 minutes, 65 deg C  
 SUBSTAGE(2) 1 hour

STAGE(2)  
 RCT AI 140373-03-1  
 RGT AK 108-48-5 2,6-Lutidine  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) 105 deg C  
 SUBSTAGE(2) 24 hours, 105 deg C  
 SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

STAGE(1)  
 RGT AH 64-18-6 HCO<sub>2</sub>H  
 SOL 7732-18-5 Water  
 CON 5 hours, 40 deg C

STAGE(2)  
 RGT D 7732-18-5 Water  
 CON 3 hours

PRO AB 140373-09-7

RX(7) RCT AB 140373-09-7

STAGE(1)  
 RGT AD 7719-09-7 SOCl<sub>2</sub>  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON SUBSTAGE(1) 30 minutes, 10 deg C  
 SUBSTAGE(2) 10 deg C -> 20 deg C

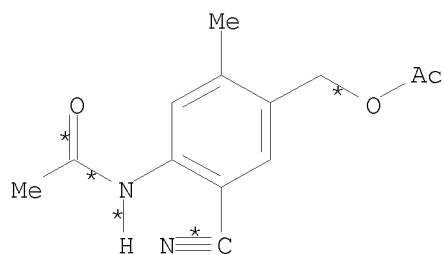
STAGE(2)  
 RCT AC 127105-49-1  
 RGT AE 7087-68-5 EtN(Pr-i)<sub>2</sub>  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON SUBSTAGE(1) 3 hours, 10 deg C  
 SUBSTAGE(2) 16 hours

STAGE(3)  
 RGT E 64-19-7 AcOH

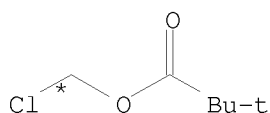
PRO W 247904-63-8  
 NTE inert

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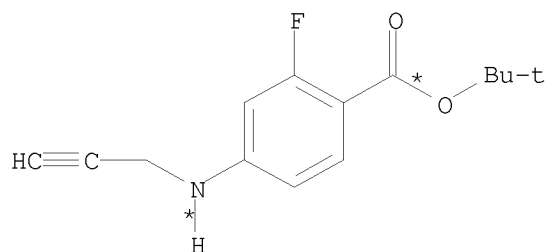
RX(38) OF 45 COMPOSED OF RX(3), RX(2), RX(1), RX(9), RX(8)  
RX(38) J + G + AI ==> AB



J

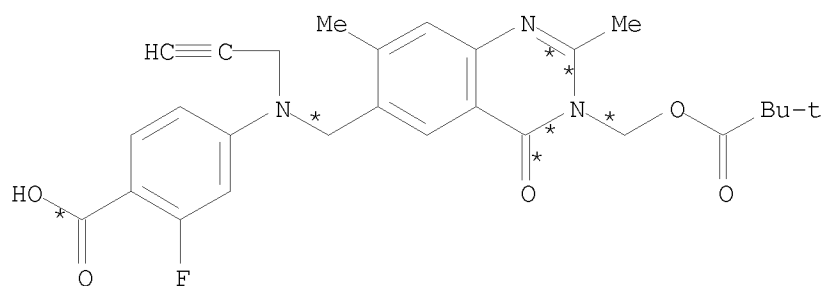


G



AI

5  
STEPS  
➤



AB

YIELD 98%

RX(3) RCT J 838858-87-0  
RGT K 7647-01-0 HCl  
PRO F 838858-86-9  
SOL 67-63-0 Me2CHOH  
CON SUBSTAGE(1) 60 minutes  
SUBSTAGE(2) 30 deg C  
NTE HCl gas used

RX(2) RCT F 838858-86-9

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STAGE(1)  
RGT H 584-08-7 K2CO3  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)  
RCT G 18997-19-8  
CON SUBSTAGE(1) 2.5 hours, 50 deg C  
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) 2 hours, 60 deg C  
SUBSTAGE(2) 3 hours, 60 deg C  
SUBSTAGE(3) 60 deg C -> 16 deg C  
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)  
RGT AJ 144-55-8 NaHCO3  
SOL 7732-18-5 Water, 108-88-3 PhMe  
CON SUBSTAGE(1) 30 minutes, 65 deg C  
SUBSTAGE(2) 1 hour

STAGE(2)  
RCT AI 140373-03-1  
RGT AK 108-48-5 2,6-Lutidine  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) 105 deg C  
SUBSTAGE(2) 24 hours, 105 deg C  
SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

STAGE(1)  
RGT AH 64-18-6 HCO2H  
SOL 7732-18-5 Water  
CON 5 hours, 40 deg C

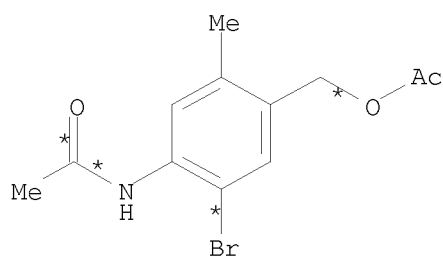
STAGE(2)  
RGT D 7732-18-5 Water  
CON 3 hours



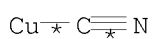
10/ 562,112

PRO AB 140373-09-7

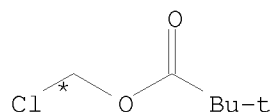
RX(39) OF 45 COMPOSED OF RX(4), RX(3), RX(2), RX(1), RX(9), RX(8)  
RX(39) M + N + G + AI ==> AB



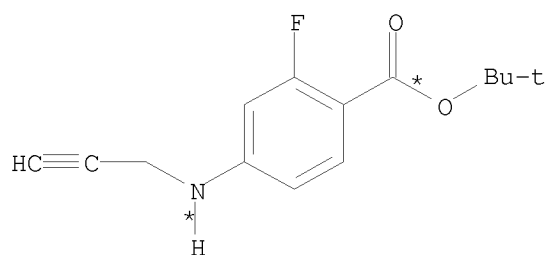
M



N

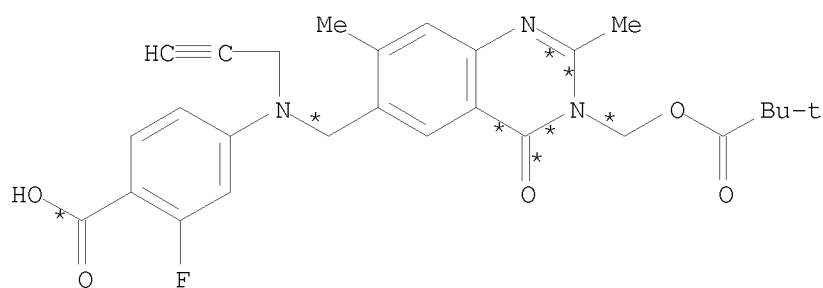


G



AI

6  
STEPS  
→



AB  
YIELD 98%

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)  
RGT O 7440-66-6 Zn  
CON SUBSTAGE(1) 60 deg C  
SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0  
NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0  
RGT K 7647-01-0 HCl  
PRO F 838858-86-9  
SOL 67-63-0 Me2CHOH  
CON SUBSTAGE(1) 60 minutes  
SUBSTAGE(2) 30 deg C  
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)  
RGT H 584-08-7 K2CO3  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)  
RCT G 18997-19-8  
CON SUBSTAGE(1) 2.5 hours, 50 deg C  
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) 2 hours, 60 deg C  
SUBSTAGE(2) 3 hours, 60 deg C  
SUBSTAGE(3) 60 deg C -> 16 deg C  
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)  
RGT AJ 144-55-8 NaHCO3  
SOL 7732-18-5 Water, 108-88-3 PhMe  
CON SUBSTAGE(1) 30 minutes, 65 deg C  
SUBSTAGE(2) 1 hour

STAGE(2)  
RCT AI 140373-03-1  
RGT AK 108-48-5 2,6-Lutidine

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SOL 108-88-3 PhMe  
CON SUBSTAGE(1) 105 deg C  
SUBSTAGE(2) 24 hours, 105 deg C  
SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

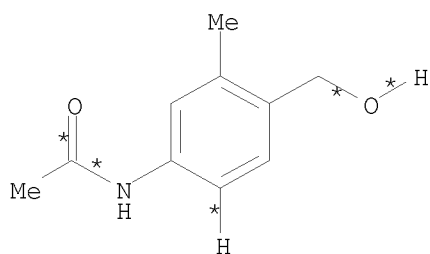
STAGE(1)  
RGT AH 64-18-6 HCO2H  
SOL 7732-18-5 Water  
CON 5 hours, 40 deg C

STAGE(2)  
RGT D 7732-18-5 Water  
CON 3 hours

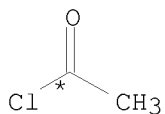
PRO AB 140373-09-7

RX(40) OF 45 COMPOSED OF RX(5), RX(4), RX(3), RX(2), RX(1), RX(9), RX(8)

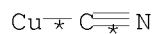
RX(40) Q + R + N + G + AI ==> AB



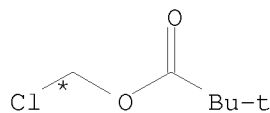
Q



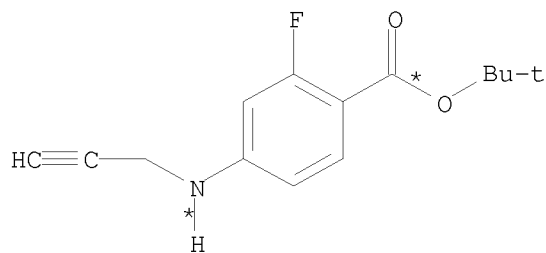
R



N



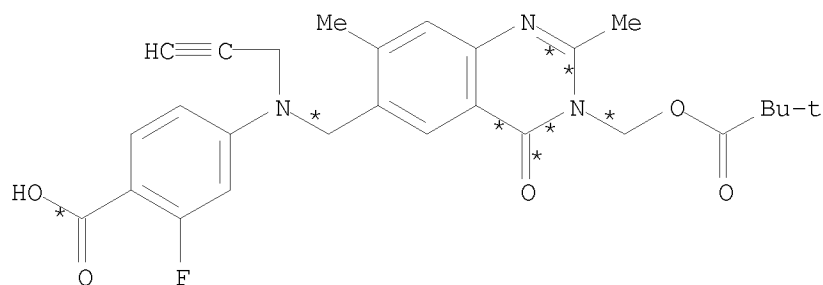
G



AI

7  
STEPS  
→

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AB  
YIELD 98%

RX(5) RCT Q 117523-91-8

STAGE(1)

RGT S 121-44-8 Et3N

SOL 141-78-6 AcOEt

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)

RCT R 75-36-5

CON SUBSTAGE(1) 2 hours, 50 deg C

SUBSTAGE(2) 30 minutes, 50 deg C

SUBSTAGE(3) 50 deg C -> 20 deg C

STAGE(3)

RGT T 1715-40-8 Bicyclo[2.2.1]hept-2-ene,  
5-(bromomethyl)-1,2,3,4,7,7-hexachloro-

SOL 75-05-8 MeCN

CON SUBSTAGE(1) 50 deg C

SUBSTAGE(2) 60 minutes

SUBSTAGE(3) 50 deg C -> 20 deg C

PRO M 838858-88-1

NTE regioselective

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0

NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0

RGT K 7647-01-0 HCl

PRO F 838858-86-9

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SOL 67-63-0 Me2CHOH  
CON SUBSTAGE(1) 60 minutes  
SUBSTAGE(2) 30 deg C  
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)  
RGT H 584-08-7 K2CO3  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)  
RCT G 18997-19-8  
CON SUBSTAGE(1) 2.5 hours, 50 deg C  
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) 2 hours, 60 deg C  
SUBSTAGE(2) 3 hours, 60 deg C  
SUBSTAGE(3) 60 deg C -> 16 deg C  
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)  
RGT AJ 144-55-8 NaHCO3  
SOL 7732-18-5 Water, 108-88-3 PhMe  
CON SUBSTAGE(1) 30 minutes, 65 deg C  
SUBSTAGE(2) 1 hour

STAGE(2)  
RCT AI 140373-03-1  
RGT AK 108-48-5 2,6-Lutidine  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) 105 deg C  
SUBSTAGE(2) 24 hours, 105 deg C  
SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

STAGE(1)  
RGT AH 64-18-6 HCO2H

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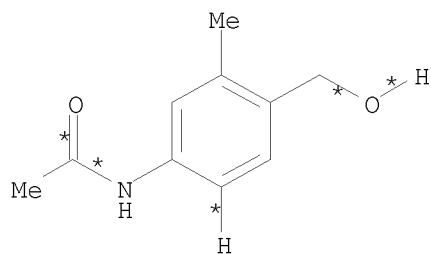
SOL 7732-18-5 Water  
CON 5 hours, 40 deg C

STAGE(2)

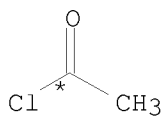
RGT D 7732-18-5 Water  
CON 3 hours

PRO AB 140373-09-7

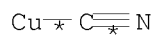
RX(41) OF 45 COMPOSED OF RX(5), RX(4), RX(3), RX(2), RX(1), RX(9), RX(8), RX(7)  
RX(41) Q + R + N + G + AI + AC ==> W



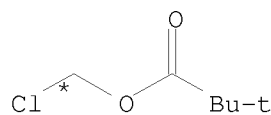
Q



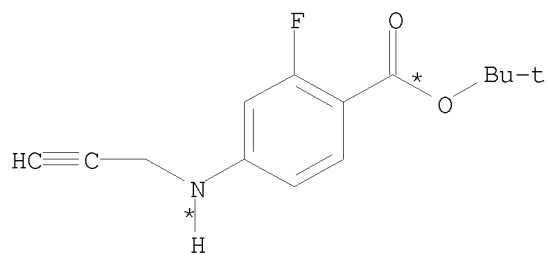
R



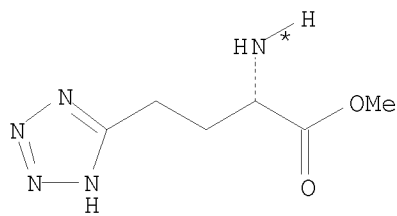
N



G



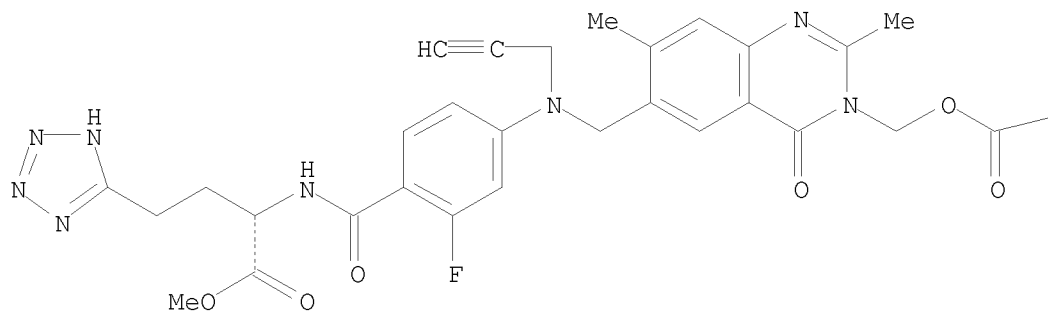
AI



AC

8

STEPS  
→



—Bu-t

W  
YIELD 82%

RX(5) RCT Q 117523-91-8

STAGE(1)

RGT S 121-44-8 Et<sub>3</sub>N  
SOL 141-78-6 AcOEt  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)

RCT R 75-36-5  
CON SUBSTAGE(1) 2 hours, 50 deg C  
SUBSTAGE(2) 30 minutes, 50 deg C  
SUBSTAGE(3) 50 deg C -> 20 deg C

STAGE(3)

RGT T 1715-40-8 Bicyclo[2.2.1]hept-2-ene,  
5-(bromomethyl)-1,2,3,4,7,7-hexachloro-  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 60 minutes  
SUBSTAGE(3) 50 deg C -> 20 deg C

PRO M 838858-88-1  
NTE regioselective

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF  
CON SUBSTAGE(1) 6 hours, 90 deg C  
SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

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RGT O 7440-66-6 Zn  
CON SUBSTAGE(1) 60 deg C  
SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0  
NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0  
RGT K 7647-01-0 HCl  
PRO F 838858-86-9  
SOL 67-63-0 Me2CHOH  
CON SUBSTAGE(1) 60 minutes  
SUBSTAGE(2) 30 deg C  
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)  
RGT H 584-08-7 K2CO3  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)  
RCT G 18997-19-8  
CON SUBSTAGE(1) 2.5 hours, 50 deg C  
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) 2 hours, 60 deg C  
SUBSTAGE(2) 3 hours, 60 deg C  
SUBSTAGE(3) 60 deg C -> 16 deg C  
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)  
RGT AJ 144-55-8 NaHCO3  
SOL 7732-18-5 Water, 108-88-3 PhMe  
CON SUBSTAGE(1) 30 minutes, 65 deg C  
SUBSTAGE(2) 1 hour

STAGE(2)  
RCT AI 140373-03-1  
RGT AK 108-48-5 2,6-Lutidine  
SOL 108-88-3 PhMe



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CON SUBSTAGE(1) 105 deg C  
SUBSTAGE(2) 24 hours, 105 deg C  
SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

STAGE(1)  
RGT AH 64-18-6 HCO2H  
SOL 7732-18-5 Water  
CON 5 hours, 40 deg C

STAGE(2)  
RGT D 7732-18-5 Water  
CON 3 hours

PRO AB 140373-09-7

RX(7) RCT AB 140373-09-7

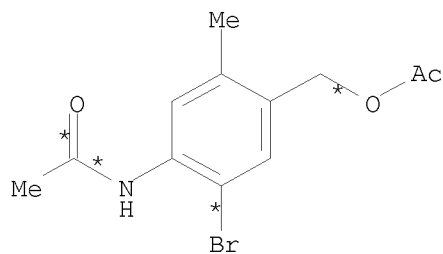
STAGE(1)  
RGT AD 7719-09-7 SOCl2  
SOL 75-09-2 CH2Cl2  
CON SUBSTAGE(1) 30 minutes, 10 deg C  
SUBSTAGE(2) 10 deg C -> 20 deg C

STAGE(2)  
RCT AC 127105-49-1  
RGT AE 7087-68-5 EtN(Pr-i)2  
SOL 75-09-2 CH2Cl2  
CON SUBSTAGE(1) 3 hours, 10 deg C  
SUBSTAGE(2) 16 hours

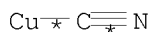
STAGE(3)  
RGT E 64-19-7 AcOH

PRO W 247904-63-8  
NTE inert

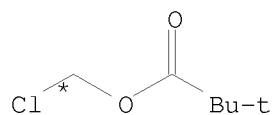
RX(42) OF 45 COMPOSED OF RX(4), RX(3), RX(2), RX(1), RX(9)  
RX(42) M + N + G + AI ==> AG



M

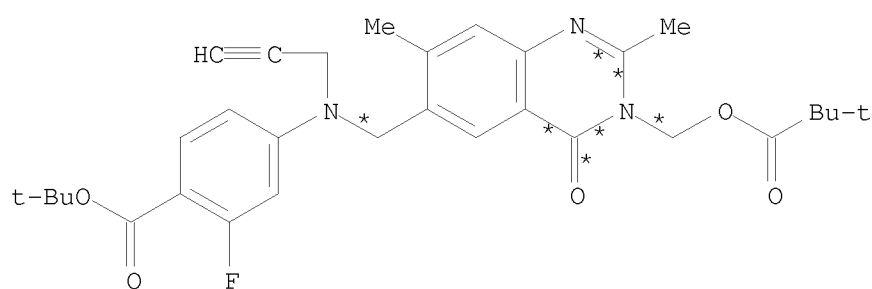
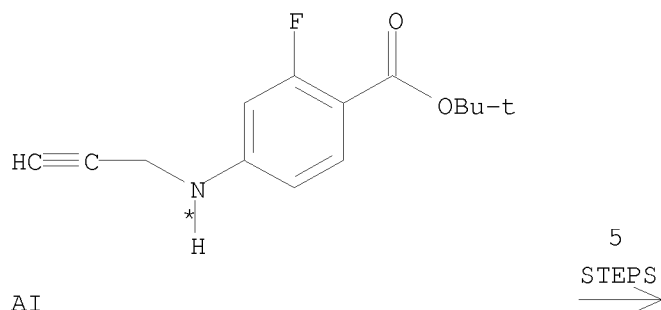


N



G

10/ 562,112



RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0

NTE inert, incremental addition of reagent in second stage

RX(3)

RCT J 838858-87-0

RGT K 7647-01-0 HCl

PRO F 838858-86-9

SOL 67-63-0 Me2CHOH

CON SUBSTAGE(1) 60 minutes

SUBSTAGE(2) 30 deg C

NTE HCl gas used

RX(2)

RCT F 838858-86-9

STAGE(1)

RGT H 584-08-7 K2CO3

SOL 67-68-5 DMSO

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CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)

RCT G 18997-19-8

CON SUBSTAGE(1) 2.5 hours, 50 deg C

SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)

RGT C 10035-10-6 HBr

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)

RGT C 10035-10-6 HBr

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) 2 hours, 60 deg C

SUBSTAGE(2) 3 hours, 60 deg C

SUBSTAGE(3) 60 deg C -> 16 deg C

SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)

RGT AJ 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water, 108-88-3 PhMe

CON SUBSTAGE(1) 30 minutes, 65 deg C

SUBSTAGE(2) 1 hour

STAGE(2)

RCT AI 140373-03-1

RGT AK 108-48-5 2,6-Lutidine

SOL 108-88-3 PhMe

CON SUBSTAGE(1) 105 deg C

SUBSTAGE(2) 24 hours, 105 deg C

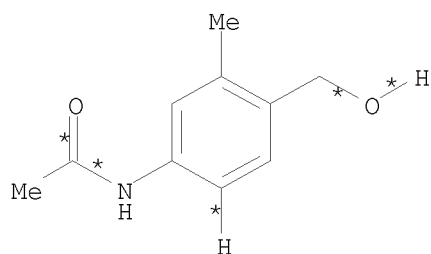
SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

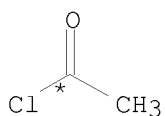
RX(43) OF 45 COMPOSED OF RX(5), RX(4), RX(3), RX(2), RX(1), RX(9)

RX(43) Q + R + N + G + AI ==> AG

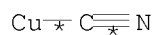
10/ 562,112



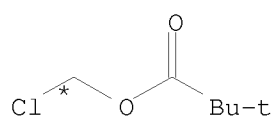
Q



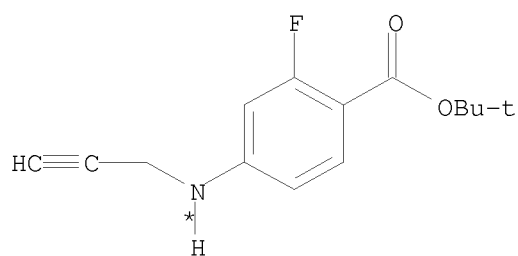
R



N

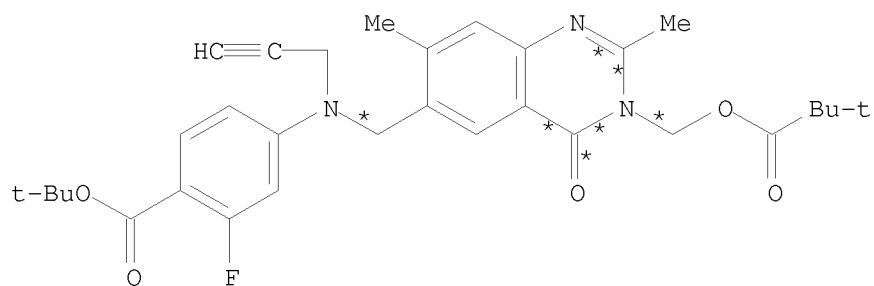


G



AI

6  
STEPS  
→



AG  
YIELD 80%

RX(5) RCT Q 117523-91-8

STAGE(1)

RGT S 121-44-8 Et3N

SOL 141-78-6 AcOEt

CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 50 deg C

## STAGE(2)

RCT R 75-36-5  
CON SUBSTAGE(1) 2 hours, 50 deg C  
SUBSTAGE(2) 30 minutes, 50 deg C  
SUBSTAGE(3) 50 deg C -> 20 deg C

## STAGE(3)

RGT T 1715-40-8 Bicyclo[2.2.1]hept-2-ene,  
5-(bromomethyl)-1,2,3,4,7,7-hexachloro-  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 60 minutes  
SUBSTAGE(3) 50 deg C -> 20 deg C

PRO M 838858-88-1  
NTE regioselective

RX(4) RCT M 838858-88-1, N 544-92-3

## STAGE(1)

SOL 68-12-2 DMF  
CON SUBSTAGE(1) 6 hours, 90 deg C  
SUBSTAGE(2) 90 deg C -> 60 deg C

## STAGE(2)

RGT O 7440-66-6 Zn  
CON SUBSTAGE(1) 60 deg C  
SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0  
NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0  
RGT K 7647-01-0 HCl  
PRO F 838858-86-9  
SOL 67-63-0 Me2CHOH  
CON SUBSTAGE(1) 60 minutes  
SUBSTAGE(2) 30 deg C  
NTE HCl gas used

RX(2) RCT F 838858-86-9

## STAGE(1)

RGT H 584-08-7 K2CO3  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 16 hours, 50 deg C

## STAGE(2)

RCT G 18997-19-8  
CON SUBSTAGE(1) 2.5 hours, 50 deg C  
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

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STAGE(1)

RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)

RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) 2 hours, 60 deg C  
SUBSTAGE(2) 3 hours, 60 deg C  
SUBSTAGE(3) 60 deg C -> 16 deg C  
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)

RGT AJ 144-55-8 NaHCO3  
SOL 7732-18-5 Water, 108-88-3 PhMe  
CON SUBSTAGE(1) 30 minutes, 65 deg C  
SUBSTAGE(2) 1 hour

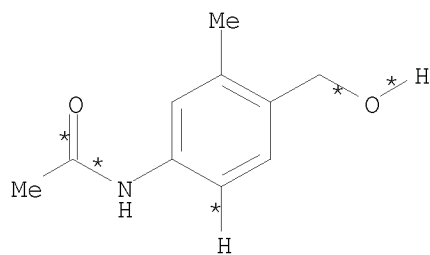
STAGE(2)

RCT AI 140373-03-1  
RGT AK 108-48-5 2,6-Lutidine  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) 105 deg C  
SUBSTAGE(2) 24 hours, 105 deg C  
SUBSTAGE(3) 105 deg C -> 65 deg C

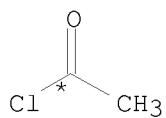
PRO AG 153538-14-8

RX(44) OF 45 COMPOSED OF RX(5), RX(4), RX(3), RX(2), RX(1)

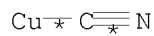
RX(44) Q + R + N + G ==> B



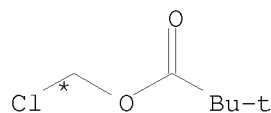
Q



R



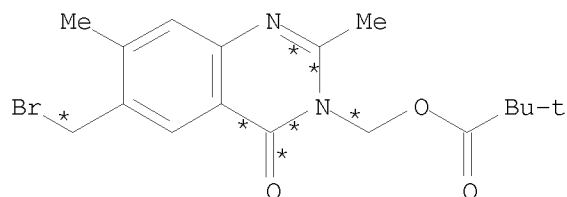
N



G

5  
STEPS  
→

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● HBr

B  
YIELD 89%

RX(5) RCT Q 117523-91-8

STAGE(1)

RGT S 121-44-8 Et3N

SOL 141-78-6 AcOEt

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)

RCT R 75-36-5

CON SUBSTAGE(1) 2 hours, 50 deg C

SUBSTAGE(2) 30 minutes, 50 deg C

SUBSTAGE(3) 50 deg C -> 20 deg C

STAGE(3)

RGT T 1715-40-8 Bicyclo[2.2.1]hept-2-ene,  
5-(bromomethyl)-1,2,3,4,7,7-hexachloro-

SOL 75-05-8 MeCN

CON SUBSTAGE(1) 50 deg C

SUBSTAGE(2) 60 minutes

SUBSTAGE(3) 50 deg C -> 20 deg C

PRO M 838858-88-1

NTE regioselective

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0

NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0

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RGT K 7647-01-0 HCl  
PRO F 838858-86-9  
SOL 67-63-0 Me2CHOH  
CON SUBSTAGE(1) 60 minutes  
SUBSTAGE(2) 30 deg C  
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)  
RGT H 584-08-7 K2CO3  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)  
RCT G 18997-19-8  
CON SUBSTAGE(1) 2.5 hours, 50 deg C  
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

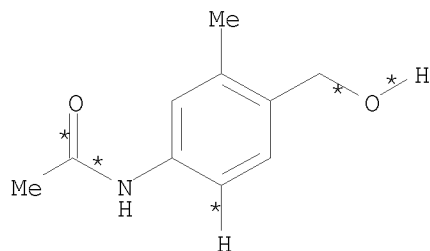
STAGE(1)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)  
RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) 2 hours, 60 deg C  
SUBSTAGE(2) 3 hours, 60 deg C  
SUBSTAGE(3) 60 deg C -> 16 deg C  
SUBSTAGE(4) 18 hours, 16 deg C

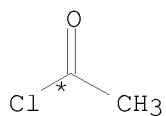
PRO B 838858-84-7

RX(45) OF 45 COMPOSED OF RX(5), RX(4), RX(3), RX(2), RX(1), RX(9), RX(8),  
RX(7), RX(6)

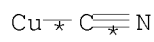
RX(45) Q + R + N + G + AI + AC ==> X



Q



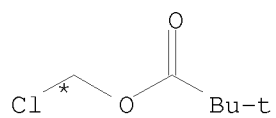
R



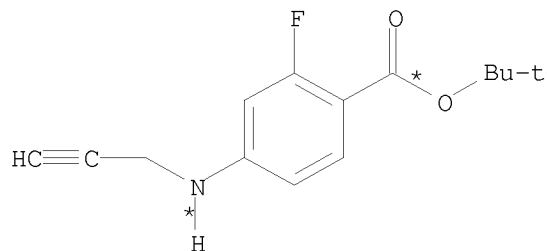
N



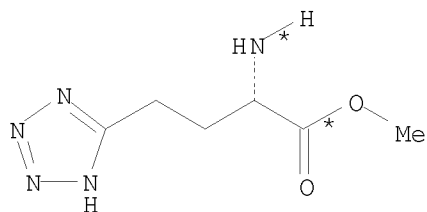
10/ 562,112



G

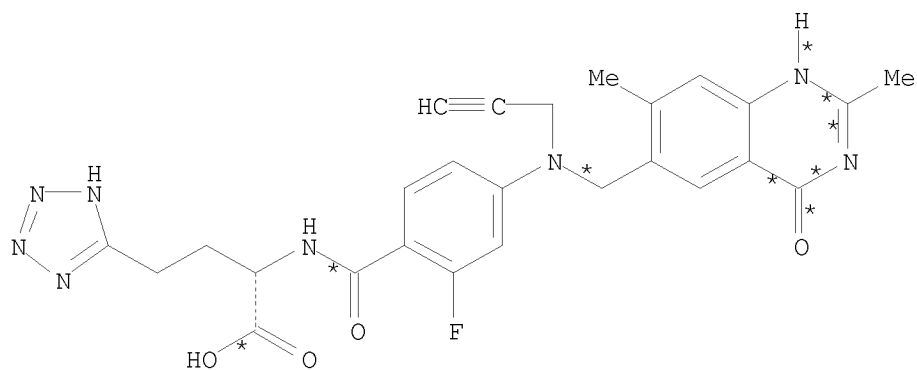


AI



AC

9  
STEPS  
→



X  
YIELD 92%

RX(5) RCT Q 117523-91-8

STAGE(1)

RGT S 121-44-8 Et3N

SOL 141-78-6 AcOEt

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)

RCT R 75-36-5

CON SUBSTAGE(1) 2 hours, 50 deg C

SUBSTAGE(2) 30 minutes, 50 deg C  
SUBSTAGE(3) 50 deg C -> 20 deg C

## STAGE(3)

RGT T 1715-40-8 Bicyclo[2.2.1]hept-2-ene,  
5-(bromomethyl)-1,2,3,4,7,7-hexachloro-  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 60 minutes  
SUBSTAGE(3) 50 deg C -> 20 deg C

PRO M 838858-88-1  
NTE regioselective

RX(4) RCT M 838858-88-1, N 544-92-3

## STAGE(1)

SOL 68-12-2 DMF  
CON SUBSTAGE(1) 6 hours, 90 deg C  
SUBSTAGE(2) 90 deg C -> 60 deg C

## STAGE(2)

RGT O 7440-66-6 Zn  
CON SUBSTAGE(1) 60 deg C  
SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0  
NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0  
RGT K 7647-01-0 HCl  
PRO F 838858-86-9  
SOL 67-63-0 Me2CHOH  
CON SUBSTAGE(1) 60 minutes  
SUBSTAGE(2) 30 deg C  
NTE HCl gas used

RX(2) RCT F 838858-86-9

## STAGE(1)

RGT H 584-08-7 K2CO3  
SOL 67-68-5 DMSO  
CON SUBSTAGE(1) 50 deg C  
SUBSTAGE(2) 16 hours, 50 deg C

## STAGE(2)

RCT G 18997-19-8  
CON SUBSTAGE(1) 2.5 hours, 50 deg C  
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

## STAGE(1)

RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 60 deg C

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STAGE(2)

RGT C 10035-10-6 HBr  
SOL 7732-18-5 Water, 64-19-7 AcOH  
CON SUBSTAGE(1) 2 hours, 60 deg C  
SUBSTAGE(2) 3 hours, 60 deg C  
SUBSTAGE(3) 60 deg C -> 16 deg C  
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)

RGT AJ 144-55-8 NaHCO<sub>3</sub>  
SOL 7732-18-5 Water, 108-88-3 PhMe  
CON SUBSTAGE(1) 30 minutes, 65 deg C  
SUBSTAGE(2) 1 hour

STAGE(2)

RCT AI 140373-03-1  
RGT AK 108-48-5 2,6-Lutidine  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) 105 deg C  
SUBSTAGE(2) 24 hours, 105 deg C  
SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

STAGE(1)

RGT AH 64-18-6 HCO<sub>2</sub>H  
SOL 7732-18-5 Water  
CON 5 hours, 40 deg C

STAGE(2)

RGT D 7732-18-5 Water  
CON 3 hours

PRO AB 140373-09-7

RX(7) RCT AB 140373-09-7

STAGE(1)

RGT AD 7719-09-7 SOCl<sub>2</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON SUBSTAGE(1) 30 minutes, 10 deg C  
SUBSTAGE(2) 10 deg C -> 20 deg C

STAGE(2)

RCT AC 127105-49-1  
RGT AE 7087-68-5 EtN(Pr-i)<sub>2</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON SUBSTAGE(1) 3 hours, 10 deg C  
SUBSTAGE(2) 16 hours

STAGE(3)

RGT E 64-19-7 AcOH

PRO W 247904-63-8

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NTE inert

RX(6) RCT W 247904-63-8

STAGE(1)

RGT Y 1310-73-2 NaOH

SOL 7732-18-5 Water, 109-99-9 THF

CON SUBSTAGE(1) 15 deg C

SUBSTAGE(2) 15 deg C -> 24 deg C

SUBSTAGE(3) 19 hours, 24 deg C

STAGE(2)

RGT Z 7631-90-5 NaHSO3

SOL 7732-18-5 Water

CON 40 minutes, 24 deg C

PRO X 153537-73-6

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 58 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 142:178643 CASREACT

TITLE: Synthesis and fastness properties of styryl and azo  
disperse dyes derived from 6-nitro substituted  
3-aryl-2-methyl-4(3H)-quinazolinone

AUTHOR(S): Bhatti, Harjinder Singh; Seshadri, Sambamurthy

CORPORATE SOURCE: Dyes Research Laboratory, University Institute of  
Chemical Technology, University of Mumbai, Mumbai,  
400019, India

SOURCE: Coloration Technology (2004), 120(4), 151-155

CODEN: CTOEAZ; ISSN: 1472-3581

PUBLISHER: Society of Dyers and Colourists

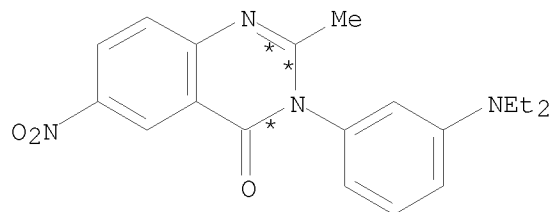
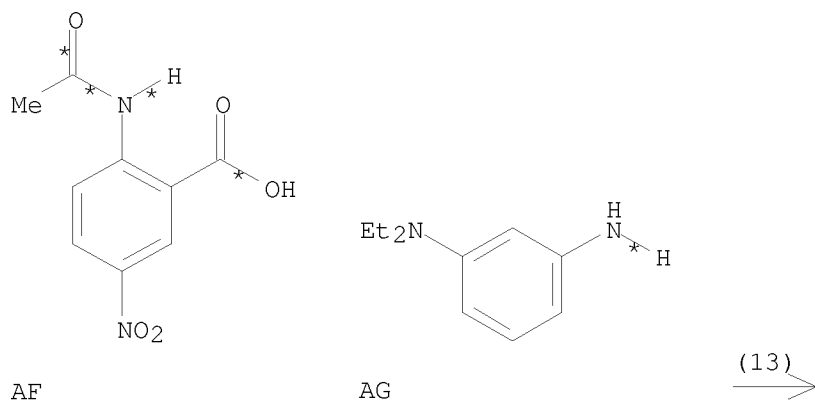
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis of 6-nitro-substituted 3-aryl-2-methyl-4(3H)-quinazolinones  
from readily available starting materials, such as isatoic anhydride, is  
described. One of these, 3-phenyl-2-methyl-4(3H)-quinazolinone, has been  
utilized to prepare a range of styryl disperse dyes for polyester. Novel  
azo disperse dyes based on 6-nitro-3-[m-(diethylamino)phenyl]-2-methyl-  
4(3H)-quinazolinone as coupling component are reported. The application  
properties of the dyes on polyester and their fastness properties have  
been evaluated, with the latter being disappointing.

RX(13) OF 57 ...AF + AG ==> Q...

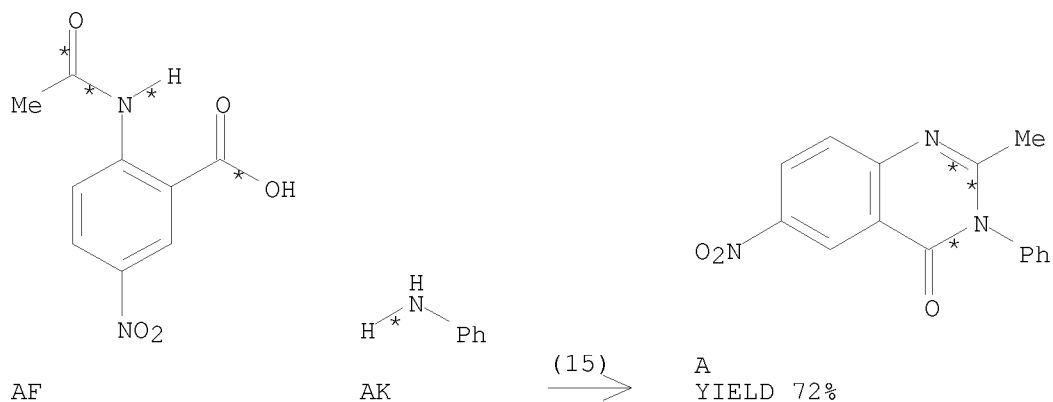
10/ 562,112



Q  
YIELD 70%

RX(13) RCT AF 3558-18-7, AG 26513-20-2  
PRO Q 834881-82-2  
NTE no exptl. detail

RX(15) OF 57 ...AF + AK ==> A...

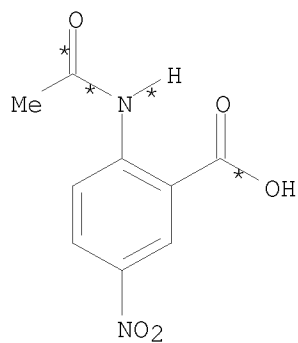


RX(15) RCT AF 3558-18-7, AK 62-53-3  
RGT AL 7719-12-2 PC13

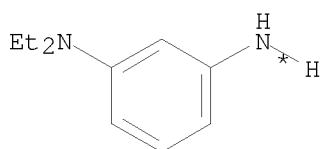
10/ 562,112

PRO A 966-91-6

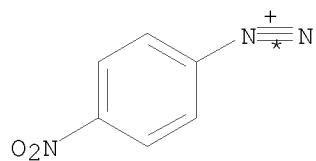
RX(17) OF 57 COMPOSED OF RX(13), RX(7)  
RX(17) AF + AG + R ==> S



AF

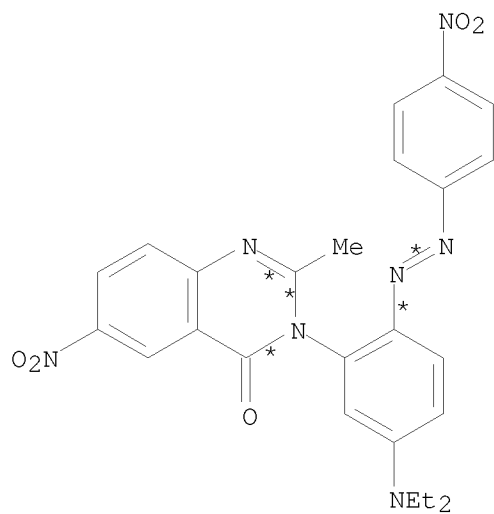


AG



R

2  
STEPS  
→



S  
YIELD 75%

RX(13) RCT AF 3558-18-7, AG 26513-20-2  
PRO Q 834881-82-2  
NTE no exptl. detail

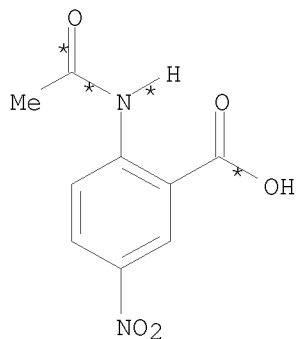
RX(7) RCT Q 834881-82-2, R 14368-49-1  
RGT T 127-09-3 AcONa  
PRO S 834881-76-4

10/ 562,112

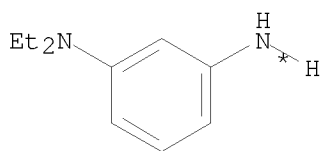
SOL 64-19-7 AcOH  
CON 2 - 3 hours, 0 - 5 deg C, pH 4 - 5  
NTE regioselective

RX(18) OF 57 COMPOSED OF RX(13), RX(8)

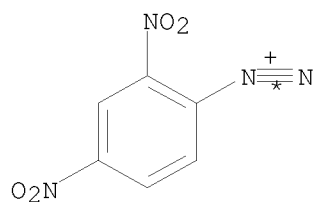
RX(18) AF + AG + V ==> W



AF

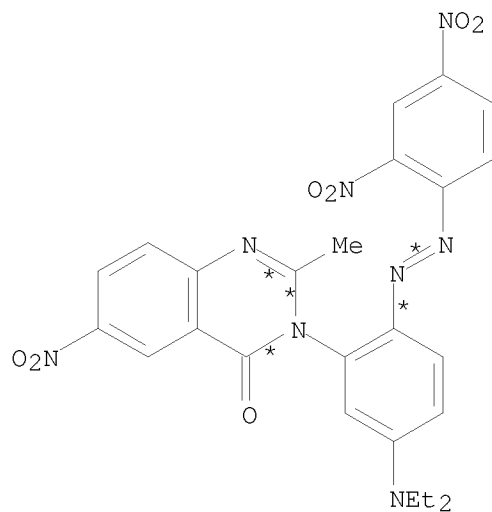


AG



V

2  
STEPS  
→



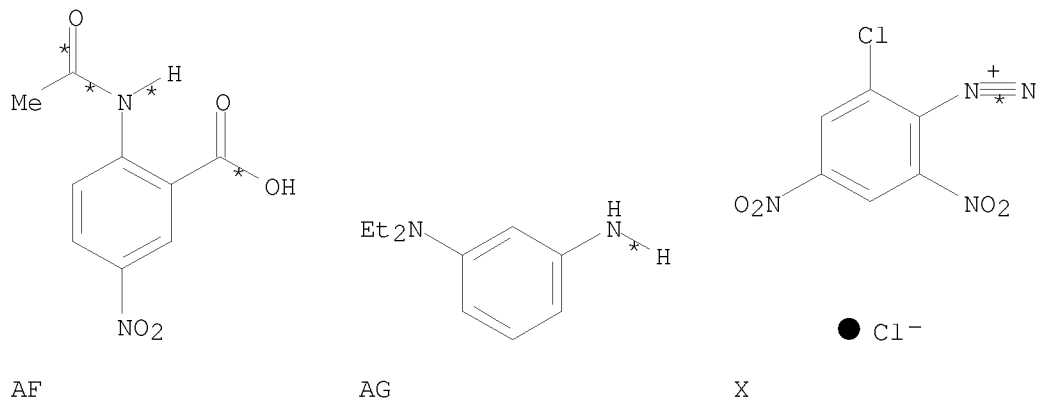
W  
YIELD 70%

RX(13) RCT AF 3558-18-7, AG 26513-20-2  
PRO Q 834881-82-2  
NTE no exptl. detail

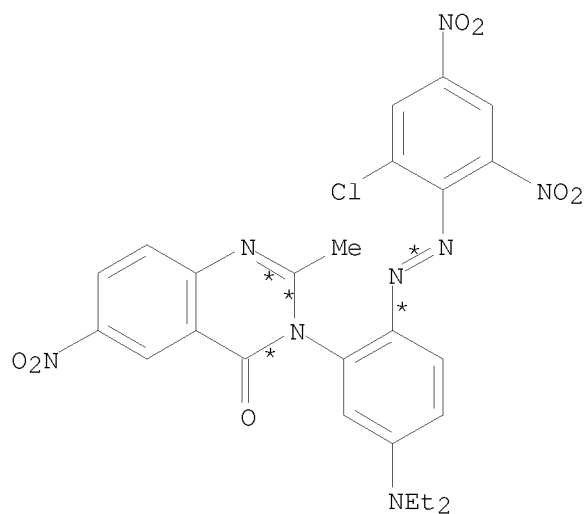
RX(8) RCT Q 834881-82-2, V 18300-85-1  
RGT T 127-09-3 AcONa  
PRO W 834881-77-5  
SOL 64-19-7 AcOH  
CON 2 - 3 hours, 0 - 5 deg C, pH 4 - 5  
NTE regioselective

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RX(19) OF 57 COMPOSED OF RX(13), RX(9)  
RX(19)      AF + AG + X ==> Y



2  
STEPS  
→



Y  
YIELD 65%

RX(13)      RCT    AF 3558-18-7, AG 26513-20-2  
              PRO    Q 834881-82-2  
              NTE    no exptl. detail

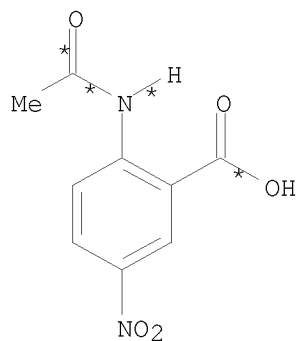
RX(9)        RCT    Q 834881-82-2, X 71668-09-2  
              RGT    T 127-09-3 AcONa  
              PRO    Y 834881-78-6  
              SOL    64-19-7 AcOH  
              CON    2 - 3 hours, 0 - 5 deg C, pH 4 - 5  
              NTE    regioselective

RX(20) OF 57 COMPOSED OF RX(13), RX(10)

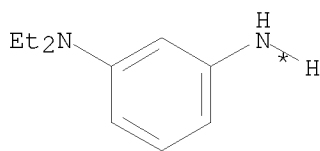


10/ 562,112

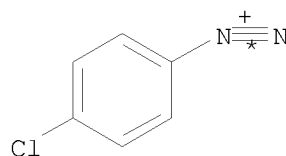
RX(20)      AF   +   AG   +   Z   ==>   AA



AF

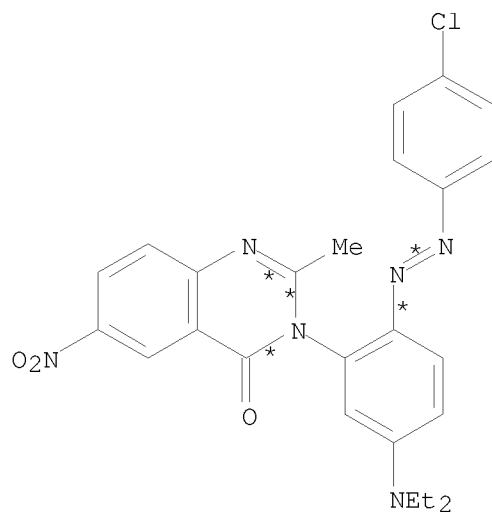


AG



Z

2  
STEPS  
→



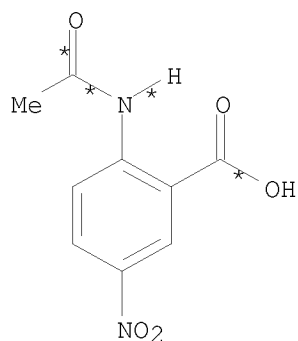
AA  
YIELD 68%

RX(13)      RCT    AF 3558-18-7, AG 26513-20-2  
              PRO    Q 834881-82-2  
              NTE    no exptl. detail

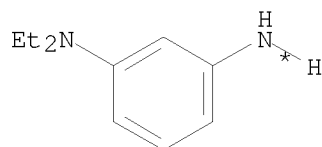
RX(10)      RCT    Q 834881-82-2, Z 17333-85-6  
              RGT    T 127-09-3 AcONa  
              PRO    AA 834881-79-7  
              SOL    64-19-7 AcOH  
              CON    2 - 3 hours, 0 - 5 deg C, pH 4 - 5  
              NTE    regioselective

RX(21) OF 57 COMPOSED OF RX(13), RX(11)  
RX(21)      AF   +   AG   +   AB   ==>   AC

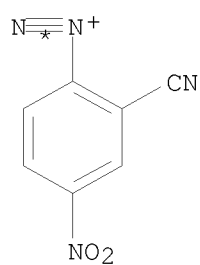
10/ 562,112



AF

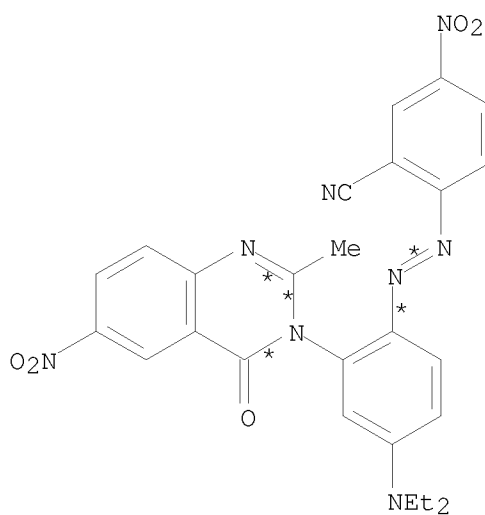


AG



AB

2  
STEPS  
→



AC  
YIELD 76%

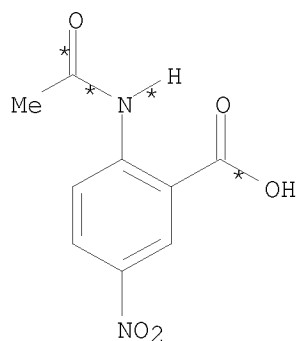
RX(13) RCT AF 3558-18-7, AG 26513-20-2  
PRO Q 834881-82-2  
NTE no exptl. detail

RX(11) RCT Q 834881-82-2, AB 66751-54-0  
RGT T 127-09-3 AcONa  
PRO AC 834881-80-0  
SOL 64-19-7 AcOH  
CON 2 - 3 hours, 0 - 5 deg C, pH 4 - 5  
NTE regioselective

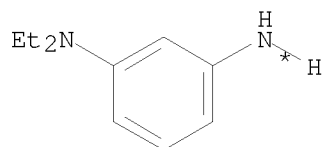
RX(22) OF 57 COMPOSED OF RX(13), RX(12)

RX(22) AF + AG + AD ==> AE

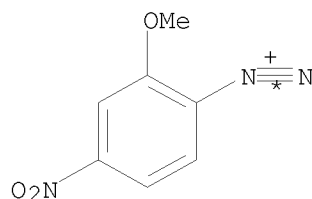
10/ 562,112



AF

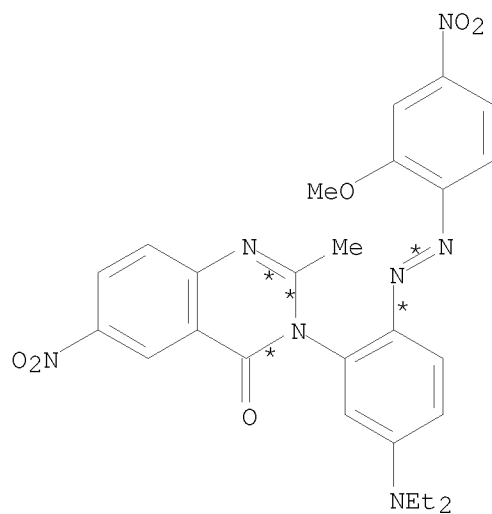


AG



AD

2  
STEPS  
→



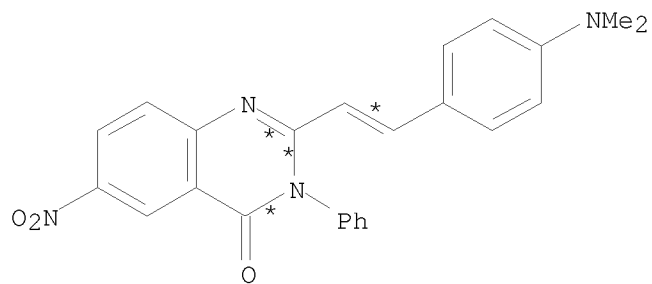
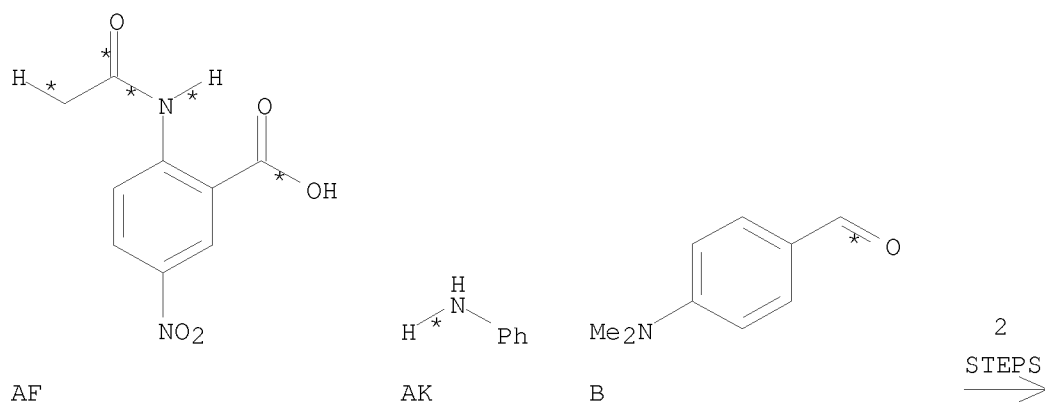
AE  
YIELD 75%

RX(13) RCT AF 3558-18-7, AG 26513-20-2  
PRO Q 834881-82-2  
NTE no exptl. detail

RX(12) RCT Q 834881-82-2, AD 27761-26-8  
RGT T 127-09-3 AcONa  
PRO AE 834881-81-1  
SOL 64-19-7 AcOH  
CON 2 - 3 hours, 0 - 5 deg C, pH 4 - 5  
NTE regioselective

RX(24) OF 57 COMPOSED OF RX(15), RX(1)  
RX(24) AF + AK + B ==> C

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C  
YIELD 76%

RX(15)      RCT    AF 3558-18-7, AK 62-53-3  
              RGT    AL 7719-12-2 PC13  
              PRO    A 966-91-6

RX(1)      RCT    A 966-91-6, B 100-10-7

STAGE(1)

RGT    D 10025-87-3 POC13

CON    SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 3 hours, reflux

SUBSTAGE(3) cooled

STAGE(2)

RGT    E 497-19-8 Na2CO3

SOL    7732-18-5 Water

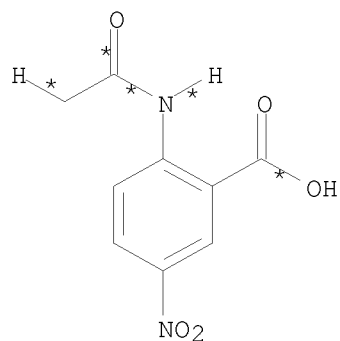
CON    pH 5

PRO    C 834881-70-8

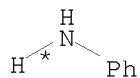
RX(25) OF 57 COMPOSED OF RX(15), RX(2)

RX(25)      AF + AK + G ==> H

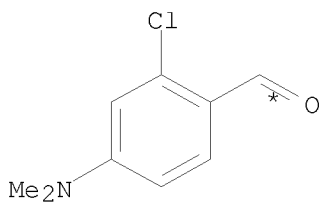
10/ 562,112



AF

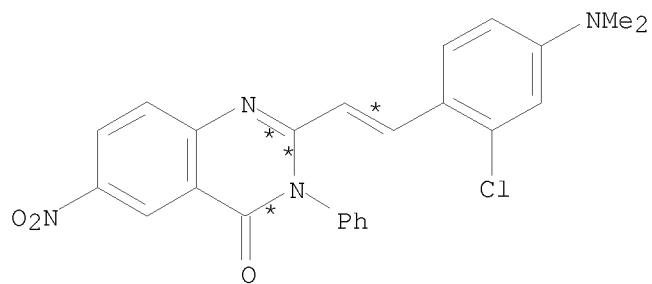


AK



G

2  
STEPS  
→



H  
YIELD 70%

RX(15) RCT AF 3558-18-7, AK 62-53-3  
RGT AL 7719-12-2 PC13  
PRO A 966-91-6

RX(2) RCT A 966-91-6, G 1424-66-4

STAGE(1)

RGT D 10025-87-3 POC13

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 3 hours, reflux

SUBSTAGE(3) cooled

STAGE(2)

RGT E 497-19-8 Na<sub>2</sub>CO<sub>3</sub>

SOL 7732-18-5 Water

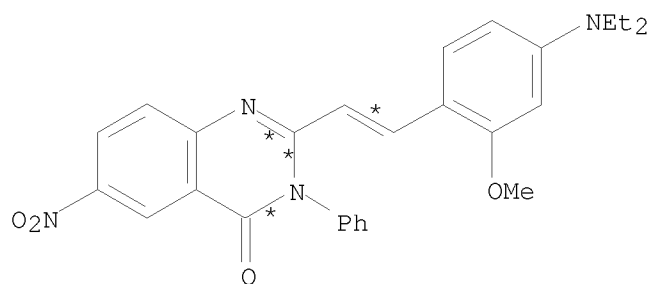
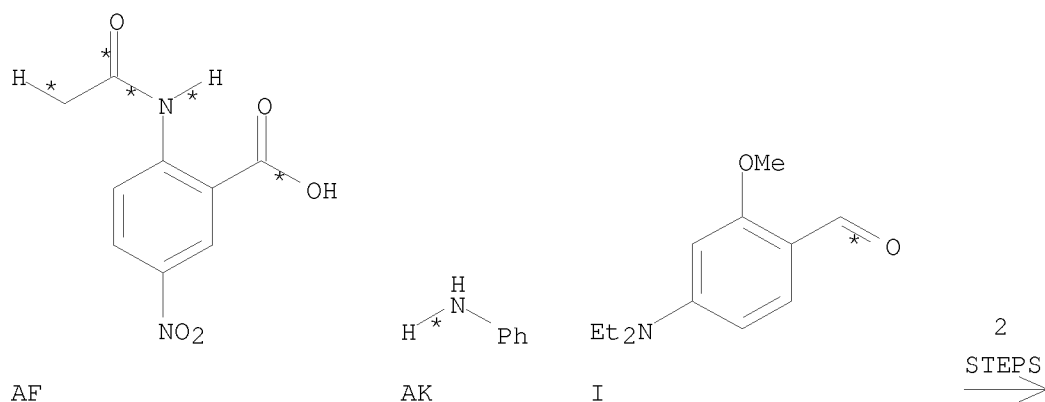
CON pH 5

PRO H 834881-71-9

RX(26) OF 57 COMPOSED OF RX(15), RX(3)

RX(26) AF + AK + I ==> J

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J  
YIELD 72%

RX(15)      RCT    AF 3558-18-7, AK 62-53-3  
              RGT    AL 7719-12-2 PC13  
              PRO    A 966-91-6

RX(3)        RCT    A 966-91-6, I 55586-68-0

STAGE(1)

RGT    D 10025-87-3 POC13  
CON    SUBSTAGE(1) room temperature -> reflux  
          SUBSTAGE(2) 3 hours, reflux  
          SUBSTAGE(3) cooled

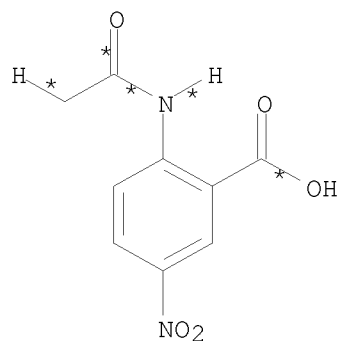
STAGE(2)

RGT    E 497-19-8 Na2CO3  
SOL    7732-18-5 Water  
CON    pH 5

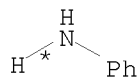
PRO    J 834881-72-0

RX(27) OF 57 COMPOSED OF RX(15), RX(4)  
RX(27)      AF + AK + K ==> L

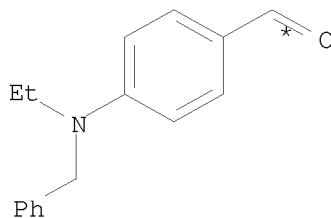
10/ 562,112



AF

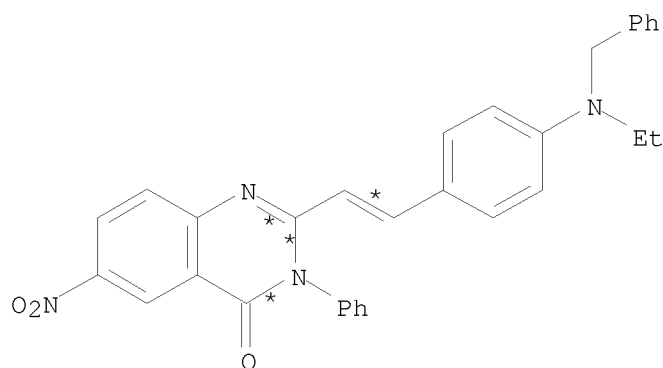


AK



K

2  
STEPS  
→



L  
YIELD 67%

RX(15) RCT AF 3558-18-7, AK 62-53-3  
RGT AL 7719-12-2 PC13  
PRO A 966-91-6

RX(4) RCT A 966-91-6, K 67676-47-5

STAGE(1)

RGT D 10025-87-3 POC13

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 3 hours, reflux

SUBSTAGE(3) cooled

STAGE(2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

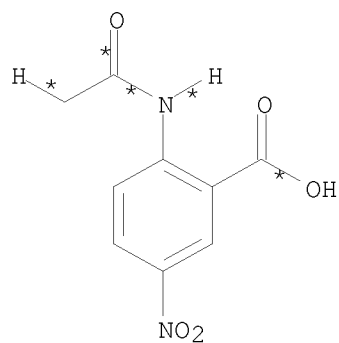
CON pH 5

PRO L 834881-73-1

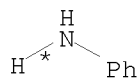
RX(28) OF 57 COMPOSED OF RX(15), RX(5)

RX(28) AF + AK + M ==> N

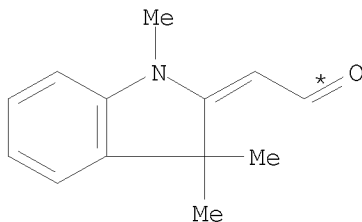
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AF

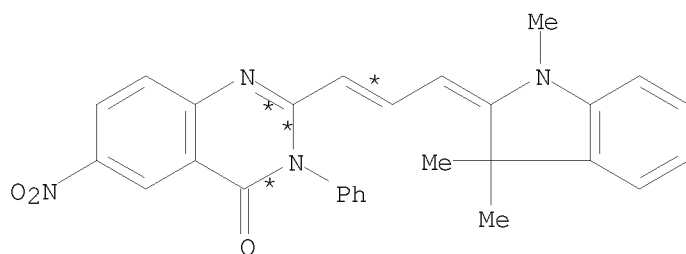


AK



M

2  
STEPS  
→



N  
YIELD 73%

RX(15) RCT AF 3558-18-7, AK 62-53-3  
RGT AL 7719-12-2 PC13  
PRO A 966-91-6

RX(5) RCT A 966-91-6, M 84-83-3

STAGE(1)

RGT D 10025-87-3 POC13

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 3 hours, reflux

SUBSTAGE(3) cooled

STAGE(2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

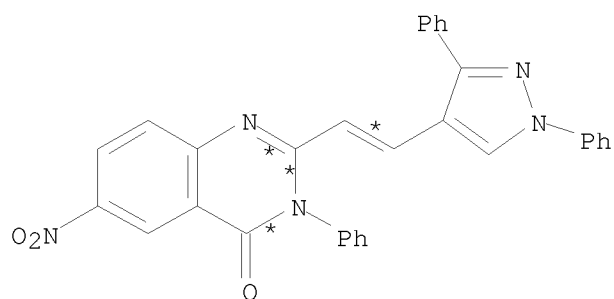
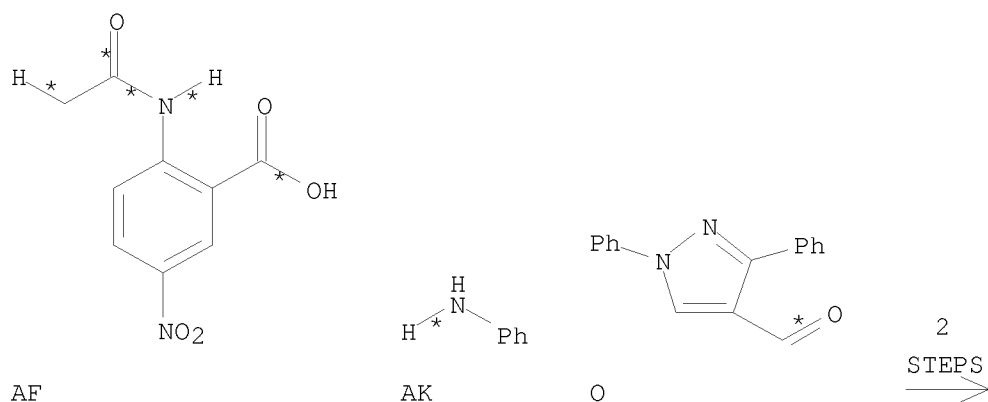
CON pH 5

PRO N 834881-74-2

RX(29) OF 57 COMPOSED OF RX(15), RX(6)

RX(29) AF + AK + O ==> P





P  
YIELD 75%

RX(15)      RCT    AF 3558-18-7, AK 62-53-3  
               RGT    AL 7719-12-2 PC13  
               PRO    A 966-91-6

RX(6) RCT A 966-91-6, O 21487-45-6

STAGE (1)

RGT D 10025-87-3 POC13

```
CON SUBSTAGE(1) room temperature -> reflux
```

SUBSTAGE (2) 3 hours, reflux

SUBSTAGE (3) cooled

STAGE (2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

CON pH 5

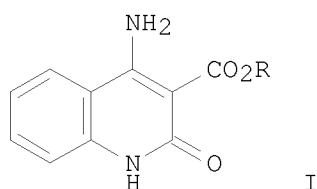
PRO P 834881-75-3

REFERENCE COUNT:

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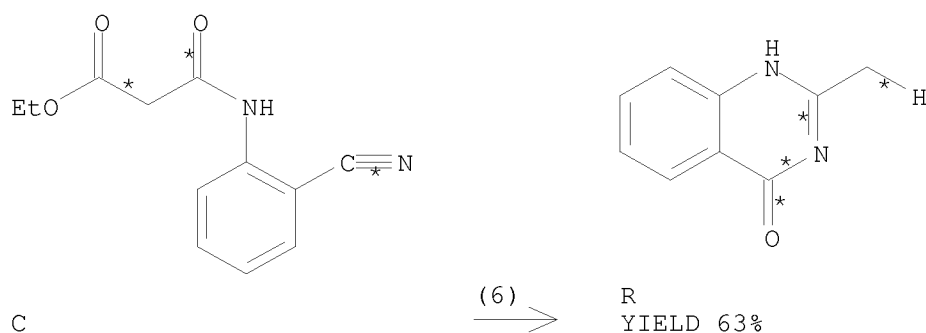
THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 59 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 142:176655 CASREACT  
 TITLE: Synthesis and structure of  
 1H-4-amino-2-oxoquinoline-3-carboxylic acid esters  
 AUTHOR(S): Ukrainets, I. V.; Bezuglyi, P. A.; Nikola, Skaif;  
 Gorokhova, O. V.; Sidorenko, L. V.  
 CORPORATE SOURCE: Nats. Farm. Univ., Kharkov, 61002, Ukraine  
 SOURCE: Zhurnal Organichnoi ta Farmatsevtichnoi Khimii (2004),  
 2(1), 39-44  
 CODEN: ZOFKAM  
 PUBLISHER: Natsional'nii Farmatsevtichnii Universitet  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 GI



AB Two approaches to the synthesis of 1H-4-amino-2-oxoquinoline-3-carboxylic acid esters I (R = Me, Et) are discussed. NMR spectroscopy studies and X-ray diffraction anal. established that these esters exist in DMSO-d6 solution and in the solid state exclusively as 4-amino-2-oxo tautomers shown.

RX(6) OF 18 ...C ==> R



RX(6) RCT C 130427-06-4

STAGE(1)

RGT Q 1310-58-3 KOH  
 SOL 7732-18-5 Water  
 CON 5 hours, reflux

STAGE(2)

RGT H 7647-01-0 HCl

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SOL 7732-18-5 Water  
CON room temperature, pH 4

PRO R 1769-24-0

L3 ANSWER 60 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 142:155910 CASREACT

TITLE: Intramolecular nucleophilic aromatic substitution  
reaction of 2-carboxamido-3-arylquinazolin-4-ones and  
its application to the synthesis of secondary aryl  
amines

AUTHOR(S): Fuwa, Haruhiko; Kobayashi, Toshitake; Tokitoh,  
Takashi; Torii, Yukiko; Natsugari, Hideaki

CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, University  
of Tokyo, Tokyo, 113-0033, Japan

SOURCE: Synlett (2004), (14), 2497-2500  
CODEN: SYNLES; ISSN: 0936-5214

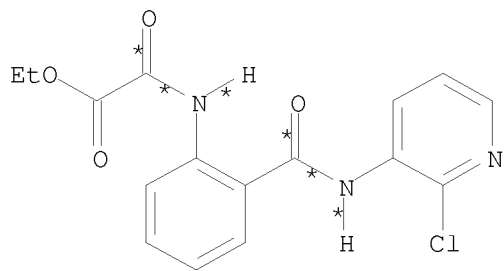
PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

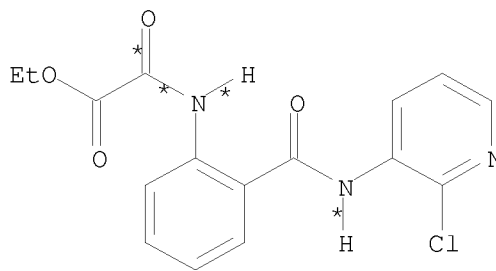
LANGUAGE: English

AB A novel intramol. nucleophilic aromatic substitution reaction of  
2-carboxamido-3-arylquinazolin-4-one derivs. induced by base treatment and  
its application to the expeditious synthesis of secondary aryl amines,  
including diaryl amines, are described.

RX(2) OF 83 ...2 C ==> F + G...



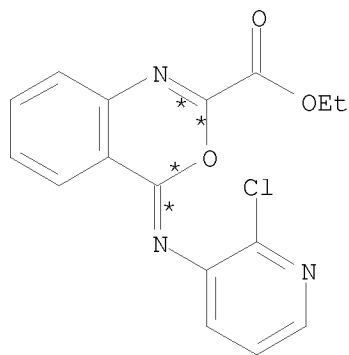
C



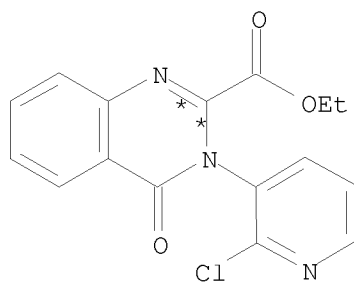
C

(2) >

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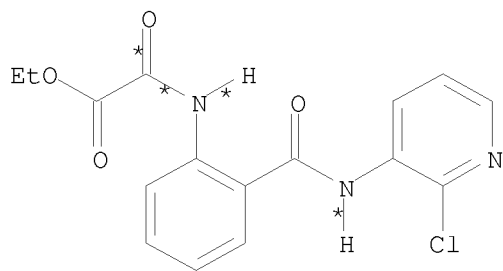
F



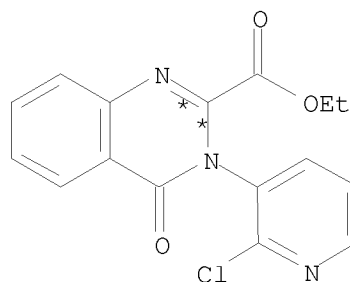
G

RX(2) RCT C 830324-66-8  
 RGT H 7087-68-5 EtN(Pr-i)2, I 7553-56-2 I2, J 603-35-0 PPh3  
 PRO F 830324-67-9, G 830324-68-0  
 SOL 75-09-2 CH2Cl2  
 CON 0 deg C -> room temperature  
 NTE Snider reaction

RX(3) OF 83 ...C ==> G...



C



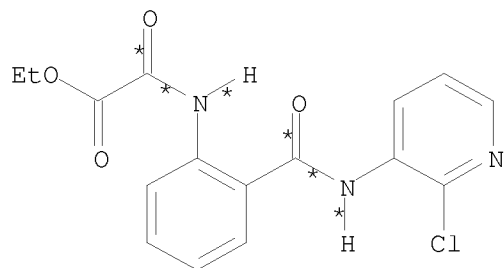
G  
YIELD 91%

RX(3) RCT C 830324-66-8  
 STAGE(1)  
 RGT H 7087-68-5 EtN(Pr-i)2, I 7553-56-2 I2, J 603-35-0 PPh3  
 SOL 75-09-2 CH2Cl2  
 CON 0 deg C -> room temperature  
 STAGE(2)  
 RGT L 123-75-1 Pyrrolidine  
 SOL 109-99-9 THF, 64-19-7 AcOH  
 CON reflux  
 PRO G 830324-68-0  
 NTE chemoselective

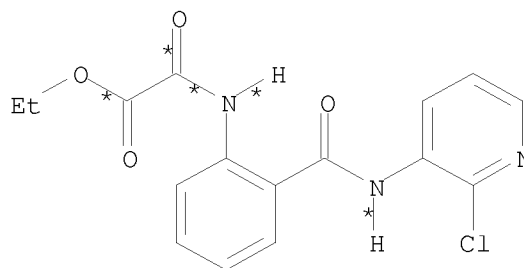
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RX(37) OF 83 COMPOSED OF RX(2), RX(4)

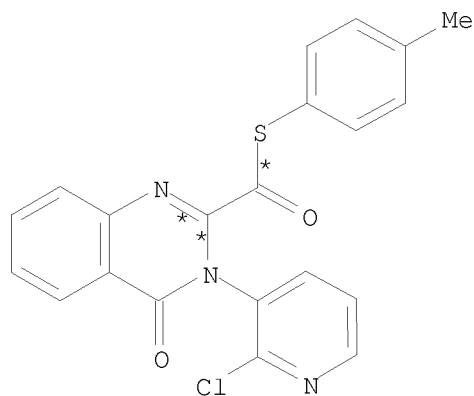
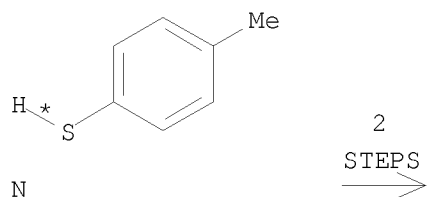
RX(37) 2 C + N ==> O



C



C



O  
YIELD 87%

RX(2) RCT C 830324-66-8  
RGT H 7087-68-5 EtN(Pr-i)<sub>2</sub>, I 7553-56-2 I<sub>2</sub>, J 603-35-0 PPh<sub>3</sub>  
PRO F 830324-67-9, G 830324-68-0  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C -> room temperature  
NTE Snider reaction

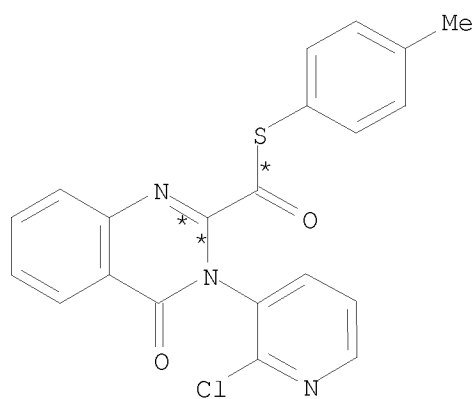
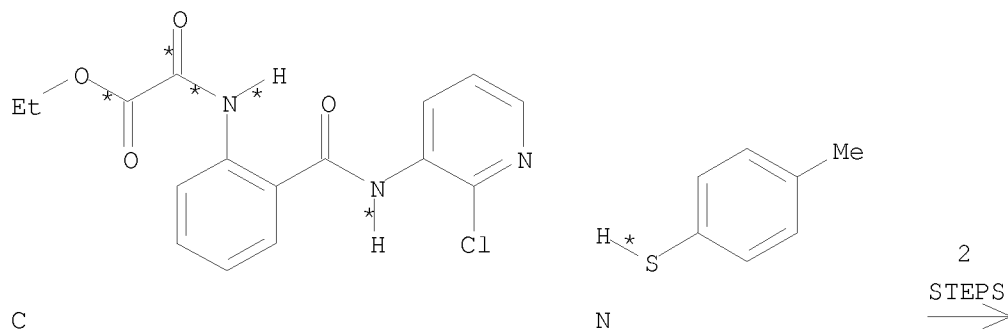
RX(4) RCT G 830324-68-0, N 106-45-6  
RGT P 75-24-1 AlMe<sub>3</sub>  
PRO O 830324-69-1  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

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CON 0 deg C -> room temperature

RX(43) OF 83 COMPOSED OF RX(3), RX(4)

RX(43) C + N ==> O



O  
YIELD 87%

RX(3) RCT C 830324-66-8

STAGE(1)

RGT H 7087-68-5 EtN(Pr-i)<sub>2</sub>, I 7553-56-2 I<sub>2</sub>, J 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON 0 deg C -> room temperature

STAGE(2)

RGT L 123-75-1 Pyrrolidine

SOL 109-99-9 THF, 64-19-7 AcOH

CON reflux

PRO G 830324-68-0

NTE chemoselective

RX(4) RCT G 830324-68-0, N 106-45-6

RGT P 75-24-1 AlMe<sub>3</sub>

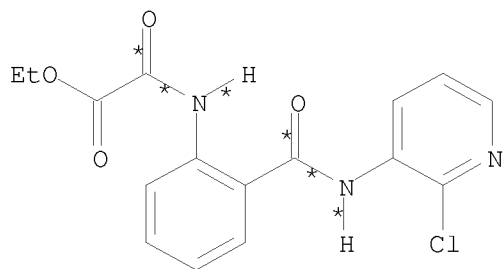
PRO O 830324-69-1

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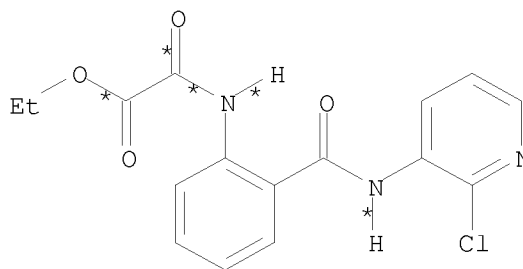
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C -> room temperature

RX(68) OF 83 COMPOSED OF RX(2), RX(4), RX(5)

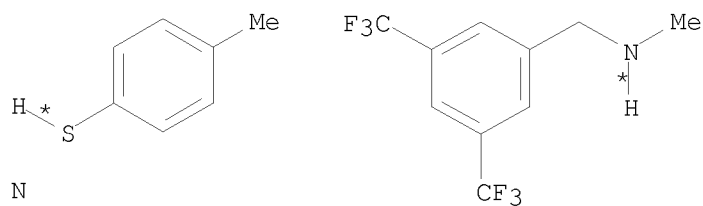
RX(68) 2 C + N + Q ==> R



C



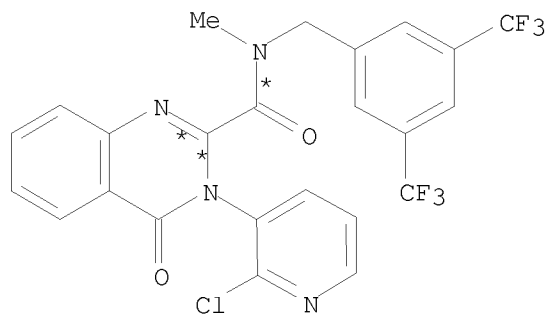
C



N

Q

3  
STEPS  
→



R  
YIELD 100%

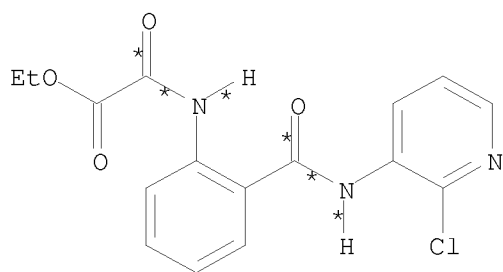
RX(2) RCT C 830324-66-8  
RGT H 7087-68-5 EtN(Pr-i)<sub>2</sub>, I 7553-56-2 I<sub>2</sub>, J 603-35-0 PPh<sub>3</sub>  
PRO F 830324-67-9, G 830324-68-0  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C -> room temperature  
NTE Snider reaction

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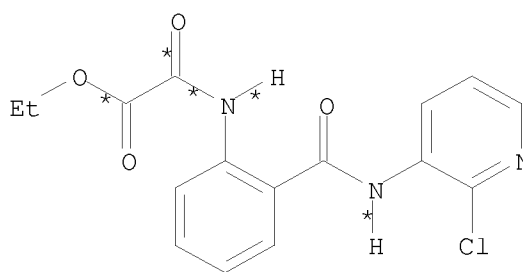
RX(4) RCT G 830324-68-0, N 106-45-6  
RGT P 75-24-1 AlMe3  
PRO O 830324-69-1  
SOL 75-09-2 CH2Cl2  
CON 0 deg C -> room temperature

RX(5) RCT O 830324-69-1, Q 159820-24-3  
RGT S 2966-50-9 F3CCO2 Ag  
PRO R 830324-71-5  
SOL 109-99-9 THF, 108-88-3 PhMe  
CON 60 deg C

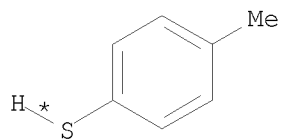
RX(69) OF 83 COMPOSED OF RX(2), RX(4), RX(6)  
RX(69) 2 C + N + U ==> V



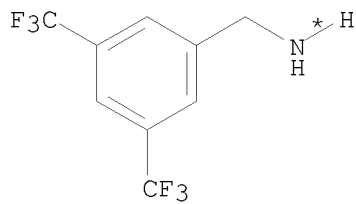
C



C



N

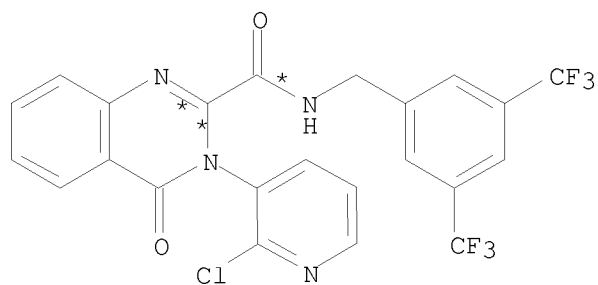


U

3  
STEPS  
→



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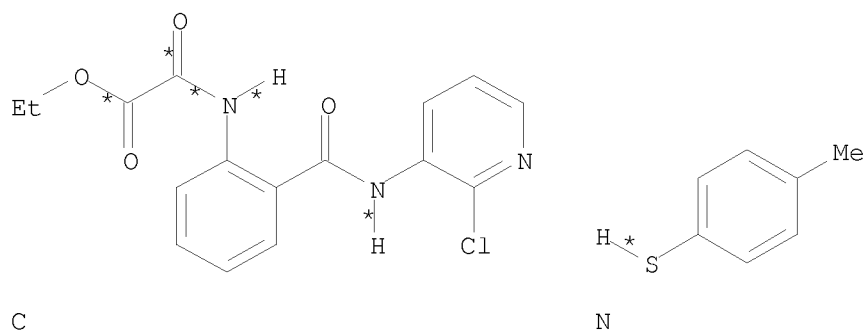
V  
YIELD 100%

RX(2) RCT C 830324-66-8  
RGT H 7087-68-5 EtN(Pr-i)2, I 7553-56-2 I2, J 603-35-0 PPh3  
PRO F 830324-67-9, G 830324-68-0  
SOL 75-09-2 CH2Cl2  
CON 0 deg C -> room temperature  
NTE Snider reaction

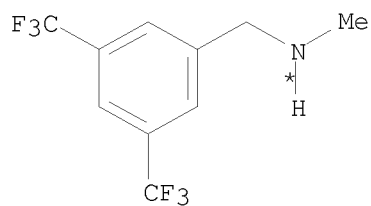
RX(4) RCT G 830324-68-0, N 106-45-6  
RGT P 75-24-1 AlMe3  
PRO O 830324-69-1  
SOL 75-09-2 CH2Cl2  
CON 0 deg C -> room temperature

RX(6) RCT O 830324-69-1, U 85068-29-7  
RGT S 2966-50-9 F3CCO2 Ag  
PRO V 830324-70-4  
SOL 109-99-9 THF, 108-88-3 PhMe  
CON 60 deg C

RX(70) OF 83 COMPOSED OF RX(3), RX(4), RX(5)  
RX(70) C + N + Q ==> R

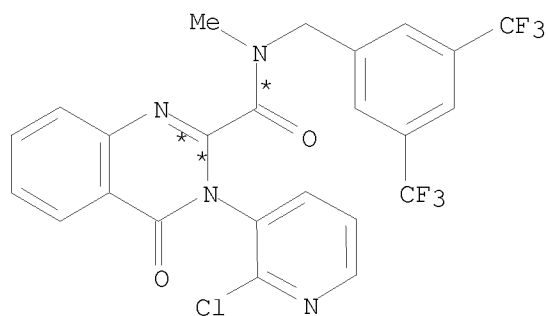


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Q

3  
STEPS  
→



R  
YIELD 100%

RX(3) RCT C 830324-66-8

STAGE(1)

RGT H 7087-68-5 EtN(Pr-i)<sub>2</sub>, I 7553-56-2 I<sub>2</sub>, J 603-35-0 PPh<sub>3</sub>

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON 0 deg C -> room temperature

STAGE(2)

RGT L 123-75-1 Pyrrolidine

SOL 109-99-9 THF, 64-19-7 AcOH

CON reflux

PRO G 830324-68-0

NTE chemoselective

RX(4) RCT G 830324-68-0, N 106-45-6

RGT P 75-24-1 AlMe<sub>3</sub>

PRO O 830324-69-1

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON 0 deg C -> room temperature

RX(5) RCT O 830324-69-1, Q 159820-24-3

RGT S 2966-50-9 F<sub>3</sub>CCO<sub>2</sub> Ag

PRO R 830324-71-5

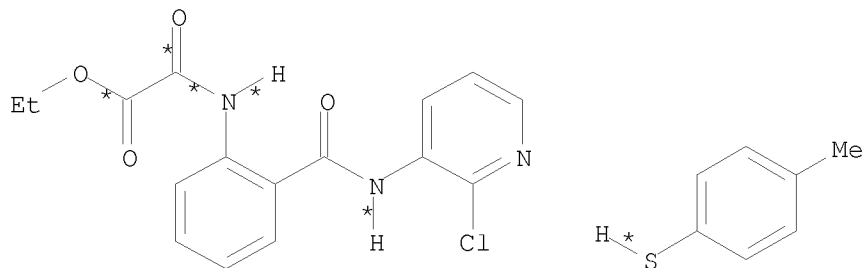
SOL 109-99-9 THF, 108-88-3 PhMe

CON 60 deg C

RX(71) OF 83 COMPOSED OF RX(3), RX(4), RX(6)

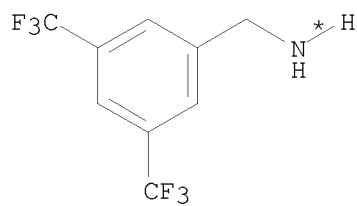
10/ 562,112

RX(71) C + N + U ==> V



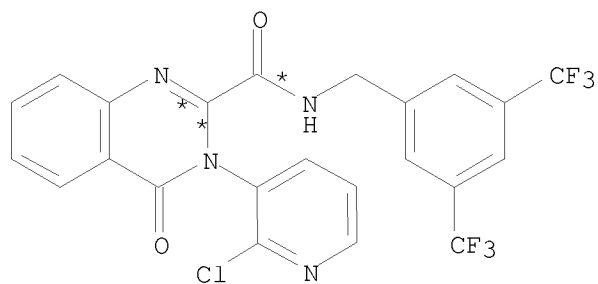
C

N



U

3  
STEPS  
➤



V  
YIELD 100%

RX(3) RCT C 830324-66-8

STAGE(1)

RGT H 7087-68-5 EtN(Pr-i)2, I 7553-56-2 I2, J 603-35-0 PPh3  
SOL 75-09-2 CH2Cl2  
CON 0 deg C -> room temperature

STAGE(2)

RGT L 123-75-1 Pyrrolidine  
SOL 109-99-9 THF, 64-19-7 AcOH  
CON reflux

PRO G 830324-68-0

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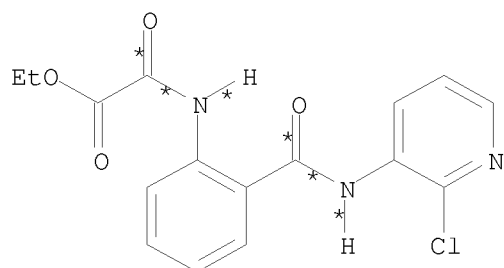
NTE chemoselective

RX(4) RCT G 830324-68-0, N 106-45-6  
 RGT P 75-24-1 AlMe3  
 PRO O 830324-69-1  
 SOL 75-09-2 CH2Cl2  
 CON 0 deg C -> room temperature

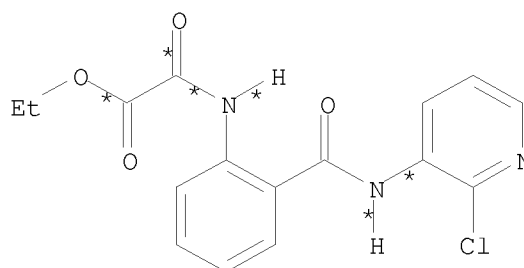
RX(6) RCT O 830324-69-1, U 85068-29-7  
 RGT S 2966-50-9 F3CCO2 Ag  
 PRO V 830324-70-4  
 SOL 109-99-9 THF, 108-88-3 PhMe  
 CON 60 deg C

RX(77) OF 83 COMPOSED OF RX(2), RX(4), RX(6), RX(7)

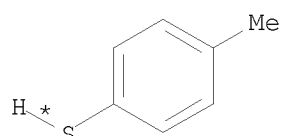
RX(77) 2 C + N + U + W ==> X



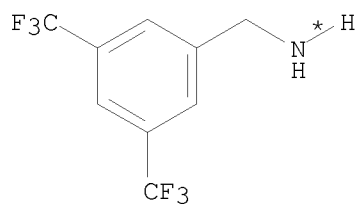
C



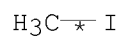
C



N



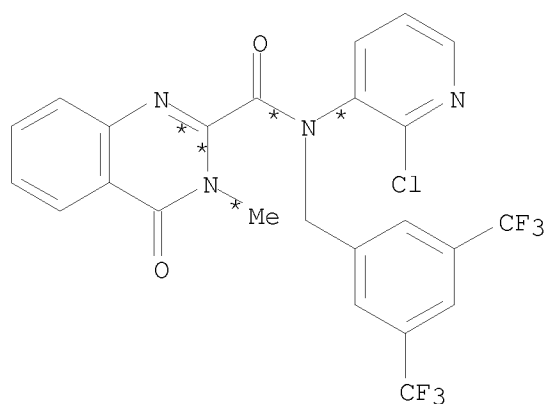
U



W

4  
 STEPS  
 →

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X  
YIELD 81%

RX(2) RCT C 830324-66-8  
RGT H 7087-68-5 EtN(Pr-i)2, I 7553-56-2 I2, J 603-35-0 PPh3  
PRO F 830324-67-9, G 830324-68-0  
SOL 75-09-2 CH2Cl2  
CON 0 deg C -> room temperature  
NTE Snider reaction

RX(4) RCT G 830324-68-0, N 106-45-6  
RGT P 75-24-1 AlMe3  
PRO O 830324-69-1  
SOL 75-09-2 CH2Cl2  
CON 0 deg C -> room temperature

RX(6) RCT O 830324-69-1, U 85068-29-7  
RGT S 2966-50-9 F3CCO2 Ag  
PRO V 830324-70-4  
SOL 109-99-9 THF, 108-88-3 PhMe  
CON 60 deg C

RX(7) RCT V 830324-70-4

STAGE(1)

RGT Y 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 1 hour, 0 deg C -> room temperature

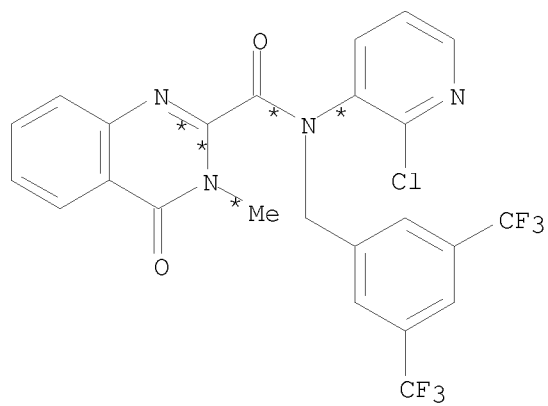
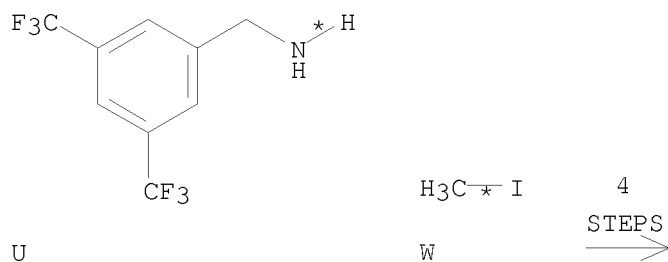
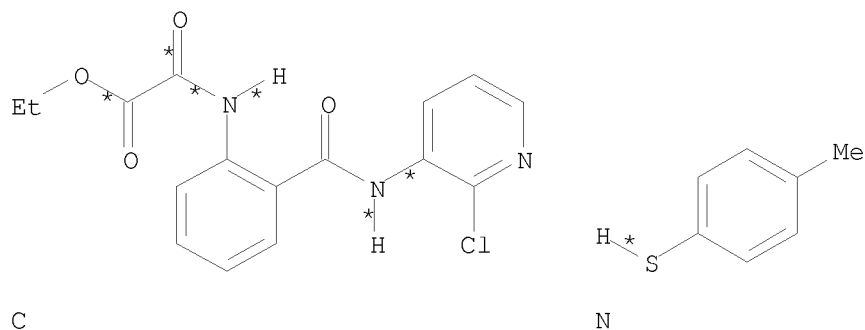
STAGE(2)

RCT W 74-88-4  
CON 1 hour, 0 deg C -> room temperature

PRO X 830324-72-6  
NTE regioselective

RX(78) OF 83 COMPOSED OF RX(3), RX(4), RX(6), RX(7)  
RX(78) C + N + U + W ==> X

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YIELD 81%

RX(3) RCT C 830324-66-8

STAGE(1)

RGT H 7087-68-5 EtN(Pr-i)2, I 7553-56-2 I2, J 603-35-0 PPh3  
SOL 75-09-2 CH2Cl2  
CON 0 deg C -> room temperature

STAGE(2)

RGT L 123-75-1 Pyrrolidine  
SOL 109-99-9 THF, 64-19-7 AcOH

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CON reflux

PRO G 830324-68-0  
NTE chemoselective

RX(4) RCT G 830324-68-0, N 106-45-6  
RGT P 75-24-1 AlMe<sub>3</sub>  
PRO O 830324-69-1  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0 deg C -> room temperature

RX(6) RCT O 830324-69-1, U 85068-29-7  
RGT S 2966-50-9 F<sub>3</sub>CCO<sub>2</sub> Ag  
PRO V 830324-70-4  
SOL 109-99-9 THF, 108-88-3 PhMe  
CON 60 deg C

RX(7) RCT V 830324-70-4

STAGE(1)

RGT Y 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 1 hour, 0 deg C -> room temperature

STAGE(2)

RCT W 74-88-4  
CON 1 hour, 0 deg C -> room temperature

PRO X 830324-72-6  
NTE regioselective

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 61 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 142:114314 CASREACT

TITLE: Intramolecular Hetero Diels-Alder (Povarov) Approach  
to the Synthesis of the Alkaloids Luotonin A and  
Camptothecin

AUTHOR(S): Twin, Heather; Batey, Robert A.

CORPORATE SOURCE: Department of Chemistry, University of Toronto,  
Toronto, ON, M5S 3H6, Can.

SOURCE: Organic Letters (2004), 6(26), 4913-4916  
CODEN: ORLEF7; ISSN: 1523-7060

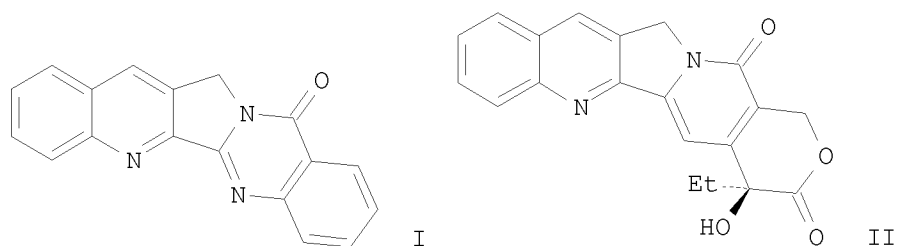
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

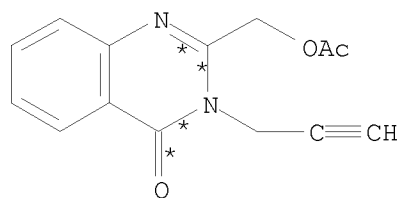
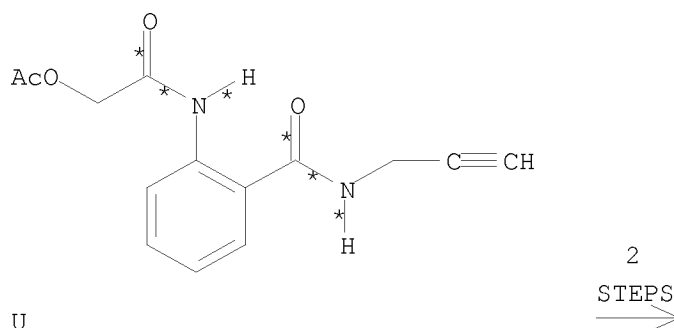
GI

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AB Pyrrolo[3,4-b]quinolines can be formed through the coupling of anilines with N-propargylic substituted heterocyclic aldehydes in the presence of mild Lewis acid catalysts. The coupling proceeds through sequential imine formation and a formal intramol. aza-Diels-Alder (Povarov) reaction. This approach was applied in a total synthesis of luotonin A (I) and a formal synthesis of camptothecin (II).

RX(19) OF 47 COMPOSED OF RX(7), RX(8)  
 RX(19) U ==> AD



YIELD 85%

RX(7) RCT U 823235-08-1

STAGE(1)

RGT Y 7087-68-5 EtN(Pr-i)2, Z 7553-56-2 I2, AA 603-35-0 PPh3  
 SOL 75-09-2 CH2Cl2  
 CON 5 hours, room temperature



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STAGE(2)

RGT AB 497-19-8 Na<sub>2</sub>CO<sub>3</sub>  
SOL 7732-18-5 Water

PRO X 823235-09-2

RX(8) RCT X 823235-09-2

STAGE(1)

RGT AE 110-89-4 Piperidine  
SOL 141-78-6 AcOEt  
CON 1 hour, room temperature

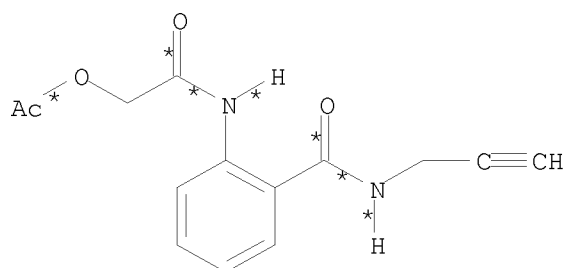
STAGE(2)

RGT AF 7631-86-9 SiO<sub>2</sub>  
SOL 141-78-6 AcOEt  
CON overnight, room temperature

PRO AD 823235-10-5

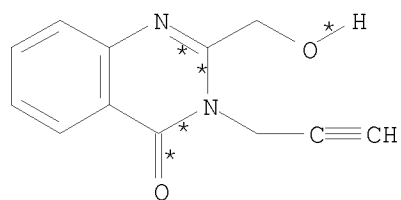
RX(33) OF 47 COMPOSED OF RX(7), RX(8), RX(13)

RX(33) U ==> AH



U

3  
STEPS  
→



AH  
YIELD 83%

RX(7) RCT U 823235-08-1

STAGE(1)

RGT Y 7087-68-5 EtN(Pr-i)<sub>2</sub>, Z 7553-56-2 I<sub>2</sub>, AA 603-35-0 PPh<sub>3</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 5 hours, room temperature

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STAGE(2)

RGT AB 497-19-8 Na2CO3  
SOL 7732-18-5 Water

PRO X 823235-09-2

RX(8) RCT X 823235-09-2

STAGE(1)

RGT AE 110-89-4 Piperidine  
SOL 141-78-6 AcOEt  
CON 1 hour, room temperature

STAGE(2)

RGT AF 7631-86-9 SiO2  
SOL 141-78-6 AcOEt  
CON overnight, room temperature

PRO AD 823235-10-5

RX(13) RCT AD 823235-10-5

STAGE(1)

RGT AT 1310-73-2 NaOH  
SOL 7732-18-5 Water, 109-99-9 THF  
CON 1 hour, room temperature

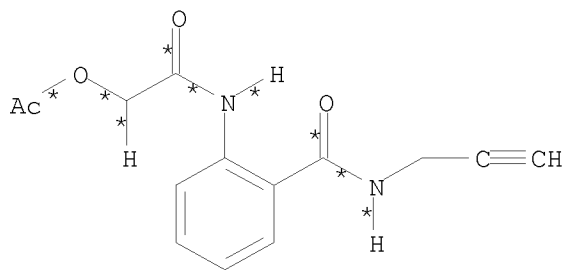
STAGE(2)

RGT O 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON pH 4.5

PRO AH 823235-13-8

RX(36) OF 47 COMPOSED OF RX(7), RX(8), RX(13), RX(9)

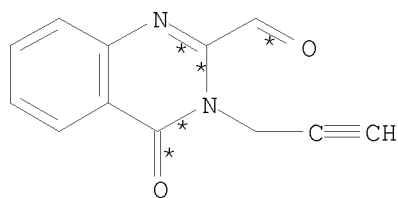
RX(36) U ==> A



U

4  
STEPS  
→

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A  
YIELD 78%

RX(7) RCT U 823235-08-1

STAGE(1)

RGT Y 7087-68-5 EtN(Pr-i)2, Z 7553-56-2 I2, AA 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON 5 hours, room temperature

STAGE(2)

RGT AB 497-19-8 Na2CO3

SOL 7732-18-5 Water

PRO X 823235-09-2

RX(8) RCT X 823235-09-2

STAGE(1)

RGT AE 110-89-4 Piperidine

SOL 141-78-6 AcOEt

CON 1 hour, room temperature

STAGE(2)

RGT AF 7631-86-9 SiO2

SOL 141-78-6 AcOEt

CON overnight, room temperature

PRO AD 823235-10-5

RX(13) RCT AD 823235-10-5

STAGE(1)

RGT AT 1310-73-2 NaOH

SOL 7732-18-5 Water, 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RGT O 7647-01-0 HCl

SOL 7732-18-5 Water

CON pH 4.5

PRO AH 823235-13-8

RX(9) RCT AH 823235-13-8

RGT AI 110-86-1 Pyridine, AJ 87413-09-0 Martin's reagent

PRO A 823235-11-6

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 15 minutes, 0 deg C

SUBSTAGE(2) 1 hour, room temperature  
 SUBSTAGE(3) 4 hours, room temperature

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 62 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 142:93763 CASREACT

TITLE: Improved synthesis of  
 3,4-dihydro-2,6-dimethyl-4-oxoquinazoline

AUTHOR(S): Chen, Shiyang; Lin, Jimao; Qin, Bingjie

CORPORATE SOURCE: School of Chemistry and Chemical Engineering, Shandong  
 University, Jinan, 250100, Peop. Rep. China

SOURCE: Organic Preparations and Procedures International  
 (2004), 36(3), 277-279

CODEN: OPPIAK; ISSN: 0030-4948

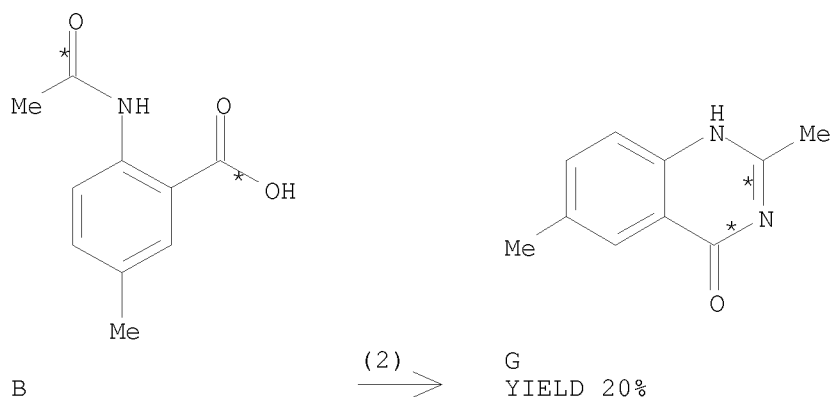
PUBLISHER: Organic Preparations and Procedures, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The preparation of title compound is described. Thus, potassium permanganate oxidation of 2,4-dimethylacetanilide gave 23% 2-acetamido-5-methylbenzoic acid which on cyclization with NH<sub>4</sub>OAc/Ac<sub>2</sub>O gave title compound

RX(2) OF 3 ...B ==> G



RX(2) RCT B 67081-68-9

STAGE(1)

SOL 108-24-7 Ac<sub>2</sub>O

CON 3 hours, reflux

STAGE(2)

RGT H 631-61-8 NH<sub>4</sub>OAc

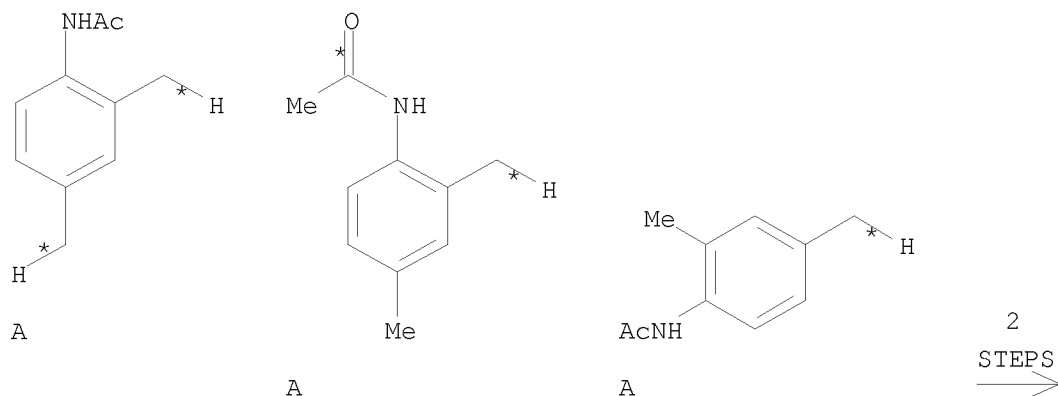
CON 16 hours, reflux

PRO G 18731-19-6

NTE petroleum ether solvent at 1st step

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RX(3) OF 3 COMPOSED OF RX(1), RX(2)  
RX(3) 3 A ==> G



G  
YIELD 20%

RX(1) RCT A 2050-43-3  
RGT E 7722-64-7 KMnO4  
PRO B 67081-68-9, C 37901-92-1, D 7501-68-0  
SOL 7732-18-5 Water  
CON 80 deg C

RX(2) RCT B 67081-68-9

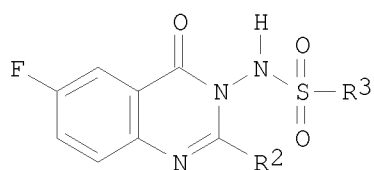
STAGE(1)  
SOL 108-24-7 Ac2O  
CON 3 hours, reflux

STAGE(2)  
RGT H 631-61-8 NH4OAc  
CON 16 hours, reflux

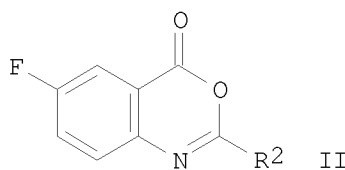
PRO G 18731-19-6  
NTE petroleum ether solvent at 1st step

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 63 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 142:23247 CASREACT  
 TITLE: Novel parallel synthesis of  
 N-(4-oxo-2-substituted-4H-quinazolin-3-yl)-substituted  
 sulfonamides  
 AUTHOR(S): Zhou, Yuefen; Murphy, Douglas E.; Sun, Zhongxiang;  
 Gregor, Vlad E.  
 CORPORATE SOURCE: Department of Medicinal Chemistry, Anadys  
 Pharmaceuticals Inc., San Diego, CA, 92121, USA  
 SOURCE: Tetrahedron Letters (2004), 45(43), 8049-8051  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



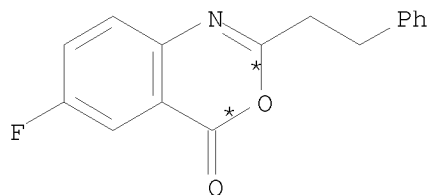
I



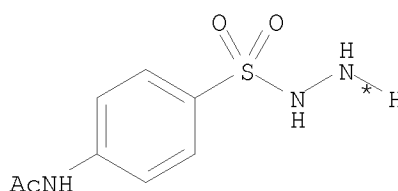
II

AB A general method was developed to synthesize a class of  
 N-(4-oxo-2-substituted-4H-quinazolin-3-yl)-substituted sulfonamides I (R2  
 = PhCH2, PhCH2CH2, 2-thiophenemethylene, R3 = 4-HO2CC6H4, 2-ClC6H4,  
 4-Me3CC6H4, etc.) in moderate to good yield by reacting benzoxazines II  
 with R3SO2NHNH2 by melting the compds. together at 130°C for 30  
 min. This new method can be applied in both single compound and parallel  
 synthesis. About 90 compds. with a variety of substituents were  
 synthesized using this method in a parallel fashion.

RX(9) OF 182 ...C + R ==> S



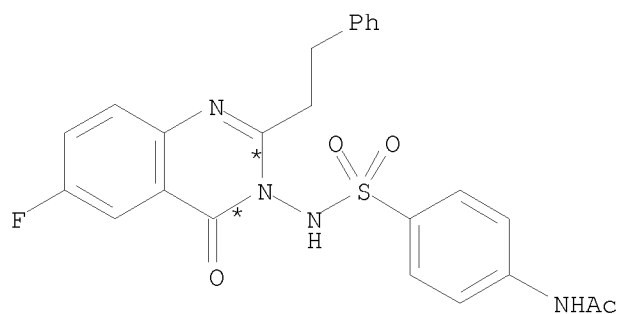
C



R

(9) >

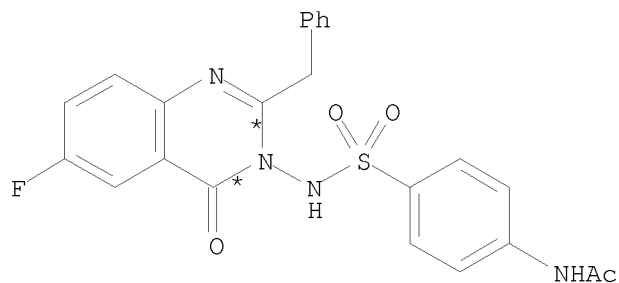
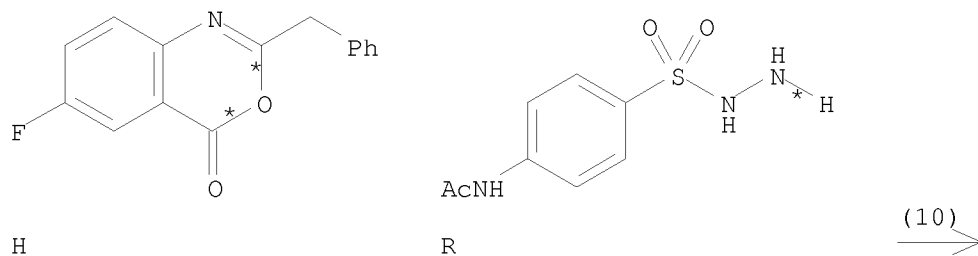
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S  
YIELD 99%

RX(9) RCT C 799797-25-4, R 3989-50-2  
PRO S 799797-38-9  
CON 30 minutes, 130 deg C  
NTE safety - potential uncontrollable decomposition, safety shield  
recommended, scale .2 mmol or smaller recommended;  
combinatorial, parallel synthesis; no solvent

RX(10) OF 182 ...H + R ==> T



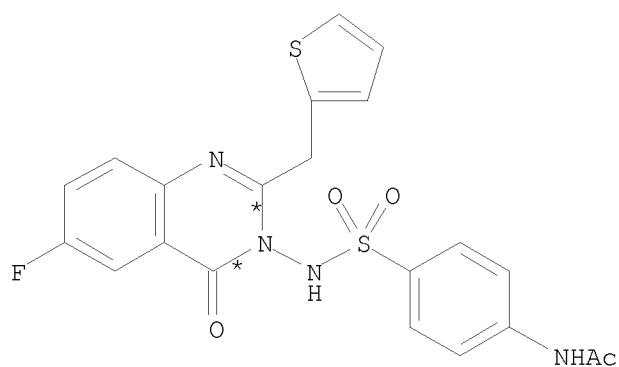
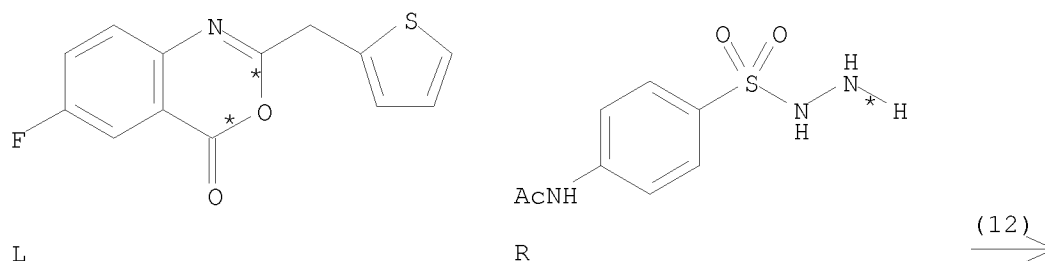
T  
YIELD 94%

RX(10) RCT H 799797-27-6, R 3989-50-2  
PRO T 799797-39-0

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CON 30 minutes, 130 deg C  
NTE safety - potential uncontrollable decomposition, safety shield  
recommended, scale .2 mmol or smaller recommended;  
combinatorial, parallel synthesis; no solvent

RX(12) OF 182 ...L + R ==> V



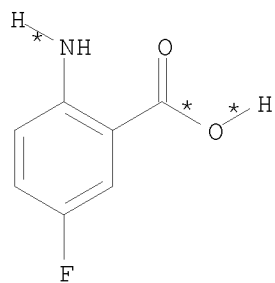
V  
YIELD 99%

RX(12) RCT L 799797-28-7, R 3989-50-2  
PRO V 799797-41-4  
CON 30 minutes, 130 deg C  
NTE safety - potential uncontrollable decomposition, safety shield  
recommended, scale .2 mmol or smaller recommended;  
combinatorial, parallel synthesis; no solvent

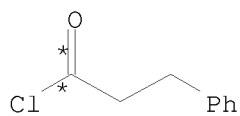
RX(95) OF 182 COMPOSED OF RX(1), RX(9)  
RX(95) A + B + R ==> S



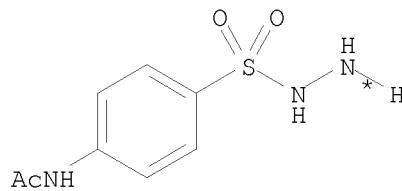
10/ 562,112



A

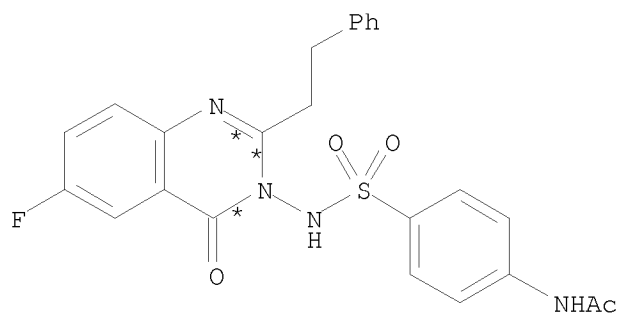


B



R

2  
STEPS  
→



S  
YIELD 99%

RX(1) RCT A 446-08-2, B 645-45-4

STAGE(1)

RGT D 121-44-8 Et<sub>3</sub>N

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON room temperature

STAGE(2)

RGT E 108-24-7 Ac<sub>2</sub>O

CON 1 hour, 165 deg C

PRO C 799797-25-4

RX(9) RCT C 799797-25-4, R 3989-50-2

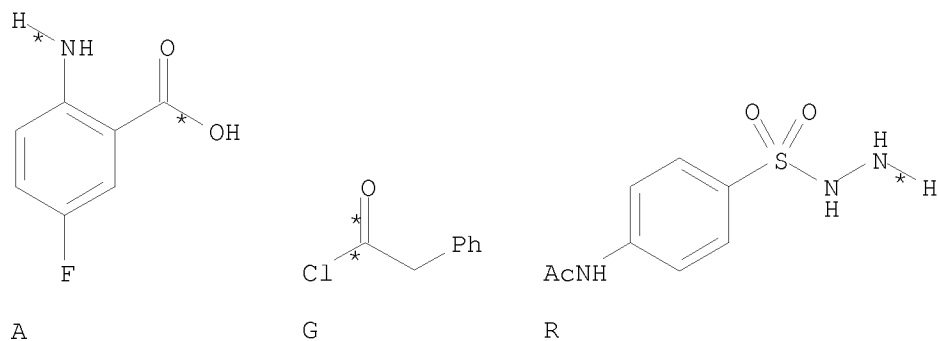
PRO S 799797-38-9

CON 30 minutes, 130 deg C

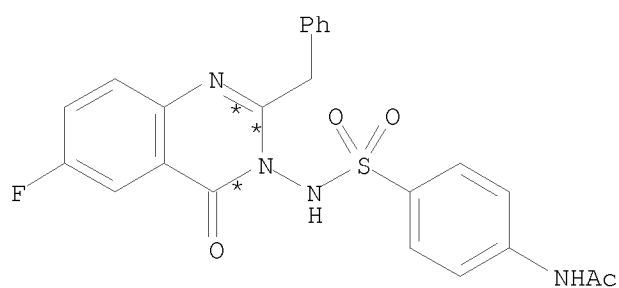
NTE safety - potential uncontrollable decomposition, safety shield recommended, scale .2 mmol or smaller recommended; combinatorial, parallel synthesis; no solvent

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RX(117) OF 182 COMPOSED OF RX(2), RX(10)  
RX(117) A + G + R ==> T



2  
STEPS  
→



T  
YIELD 94%

RX(2) RCT A 446-08-2, G 103-80-0

STAGE(1)

RGT D 121-44-8 Et3N  
SOL 75-09-2 CH2Cl2  
CON room temperature

STAGE(2)

RGT E 108-24-7 Ac2O  
CON 1 hour, 165 deg C

PRO H 799797-27-6

RX(10) RCT H 799797-27-6, R 3989-50-2

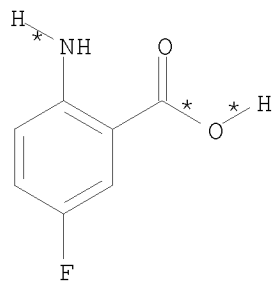
PRO T 799797-39-0

CON 30 minutes, 130 deg C

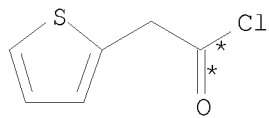
NTE safety - potential uncontrollable decomposition, safety shield  
recommended, scale .2 mmol or smaller recommended;  
combinatorial, parallel synthesis; no solvent

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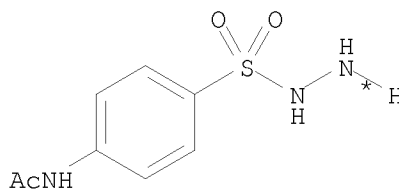
RX(160) OF 182 COMPOSED OF RX(4), RX(12)  
RX(160) A + K + R ==> V



A

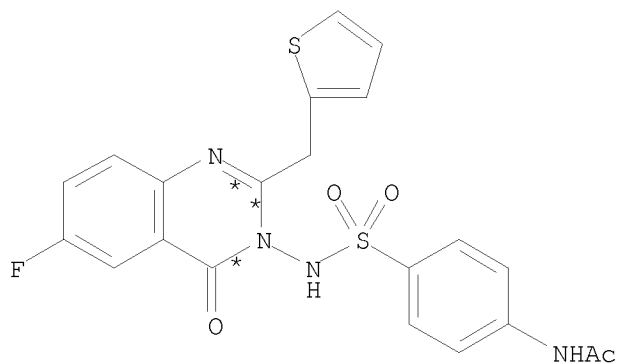


K



R

2  
STEPS  
→



V  
YIELD 99%

RX(4) RCT A 446-08-2, K 39098-97-0

STAGE(1)

RGT D 121-44-8 Et3N  
SOL 75-09-2 CH2Cl2  
CON room temperature

STAGE(2)

RGT E 108-24-7 Ac2O  
CON 1 hour, 165 deg C

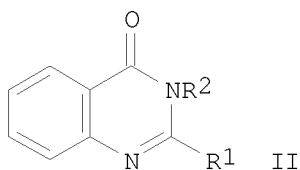
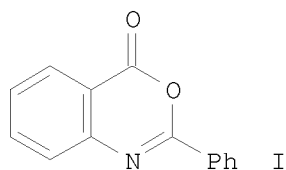
PRO L 799797-28-7

RX(12) RCT L 799797-28-7, R 3989-50-2  
PRO V 799797-41-4  
CON 30 minutes, 130 deg C

NTE safety - potential uncontrollable decomposition, safety shield recommended, scale .2 mmol or smaller recommended; combinatorial, parallel synthesis; no solvent

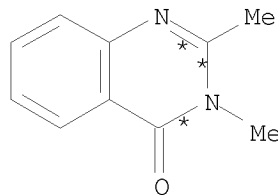
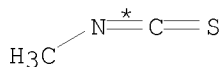
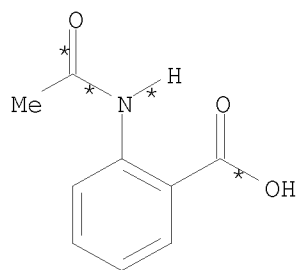
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 64 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 142:23246 CASREACT  
 TITLE: Microwave irradiated one flask synthesis of 2,3-disubstituted quinazolin-4-ones  
 AUTHOR(S): Tripathy, Pradeep K.  
 CORPORATE SOURCE: Department of Chemistry, North Eastern Regional Institute of Science and Technology, Itanagar, 791 109, India  
 SOURCE: Journal of the Institution of Chemists (India) (2003), 75(6), 179-180  
 CODEN: JOICA7; ISSN: 0020-3254  
 PUBLISHER: Institution of Chemists (India)  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Microwave-induced reaction of N-acetyl- and N-benzoylanthranilic acid with Me and Ph isothiocyanate gave benzoxazinone I and quinazolinones II (R1 = R2 = Me, Ph; R1 = Me, R2 = Ph).

RX(1) OF 4 A + B ==> C



A

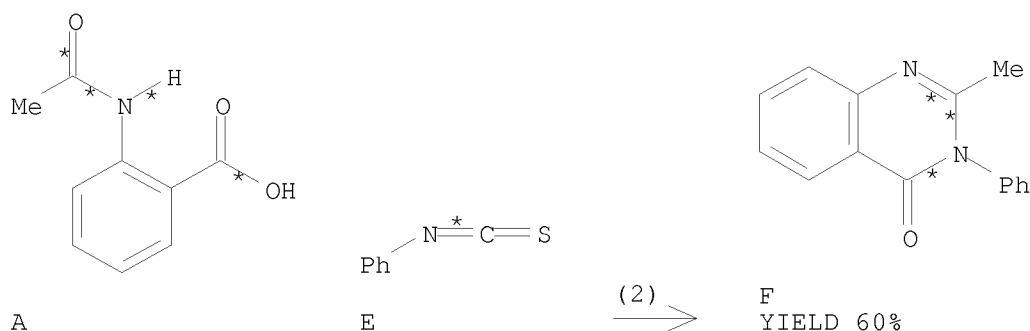
B

C  
YIELD 35%

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RX(1) RCT A 89-52-1, B 556-61-6  
PRO C 1769-25-1  
CAT 110-86-1 Pyridine  
CON 5 minutes  
NTE microwave irradiation, no solvent

RX(2) OF 4 A + E ==> F



RX(2) RCT A 89-52-1, E 103-72-0  
PRO F 2385-23-1  
CAT 110-86-1 Pyridine  
CON 5 minutes  
NTE microwave irradiation, no solvent

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 65 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 141:366195 CASREACT

TITLE: Benzenesulfonyl chloride as a cyclocondensing agent in one pot synthesis of 3-substituted 2-methylquinazolin-4-ones

AUTHOR(S): Tripathy, Pradeep K.

CORPORATE SOURCE: Department of Chemistry, North Eastern Regional Institute of Science & Technology, Itanagar, 791 109, India

SOURCE: Journal of the Institution of Chemists (India) (2004), 76(1), 6-8

CODEN: JOICA7; ISSN: 0020-3254

PUBLISHER: Institution of Chemists (India)

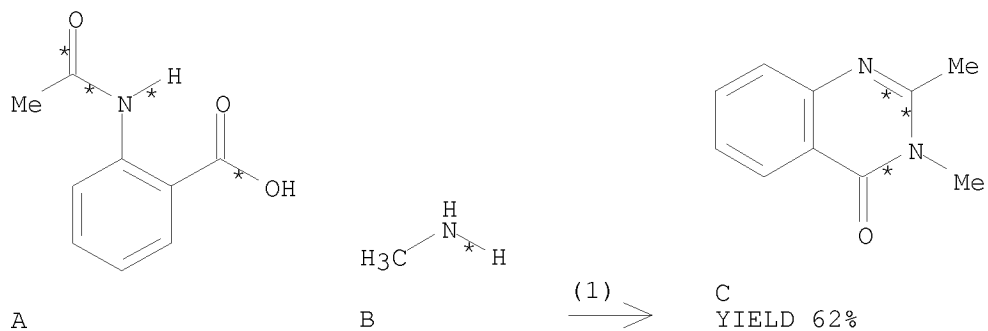
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The objective of the present study was to develop a method for the rapid and facile synthesis of 3-substituted 2-methyl-quinazolin-4-ones by using benzenesulfonyl chloride as cyclocondensing agent. Benzenesulfonyl chloride is easily available as an effective cyclocondensing agent for N-acetylglutathione. Considering the easy availability of the starting materials, speed of the reaction, the mild exptl. conditions and the simplicity of the workup, the present method appears to be useful.

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RX(1) OF 3      A + B ==> C



RX(1)      RCT    A 89-52-1

STAGE(1)

RGT   D 98-09-9 PhSO<sub>2</sub>Cl, E 121-44-8 Et<sub>3</sub>N

SOL   71-43-2 Benzene

CON   room temperature

STAGE(2)

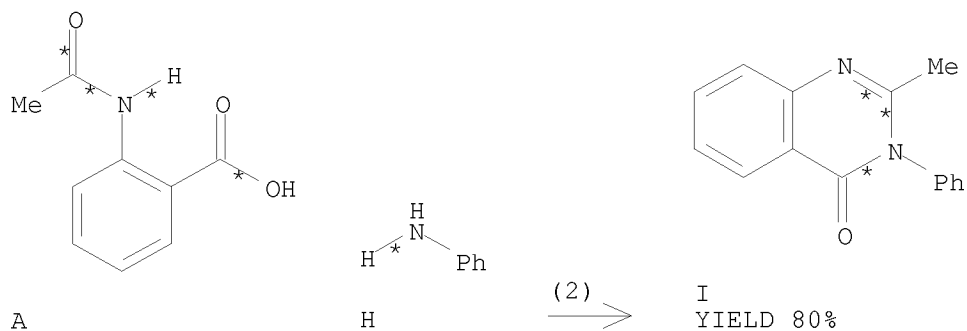
RCT   B 74-89-5

SOL   64-19-7 AcOH

CON   4 hours, reflux

PRO   C 1769-25-1

RX(2) OF 3      A + H ==> I



RX(2)      RCT    A 89-52-1

STAGE(1)

RGT   D 98-09-9 PhSO<sub>2</sub>Cl, E 121-44-8 Et<sub>3</sub>N

SOL   71-43-2 Benzene

CON   room temperature

STAGE(2)

RCT   H 62-53-3

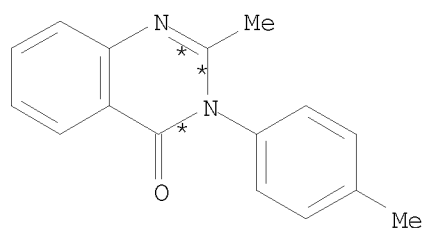
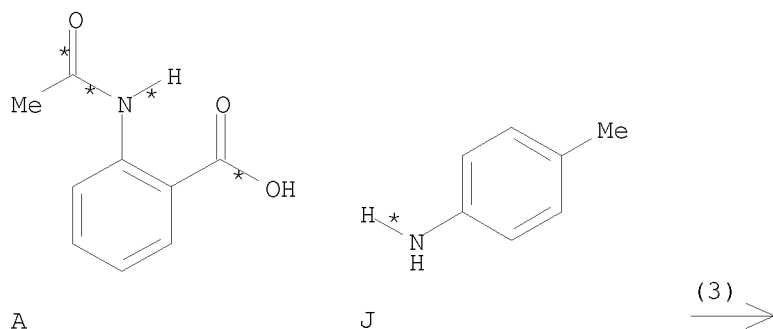
SOL   64-19-7 AcOH

CON   4 hours, reflux

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PRO I 2385-23-1

RX(3) OF 3 A + J ==> K



K  
YIELD 78%

RX(3) RCT A 89-52-1

STAGE(1)

RGT D 98-09-9 PhSO<sub>2</sub>Cl, E 121-44-8 Et<sub>3</sub>N  
SOL 71-43-2 Benzene  
CON room temperature

STAGE(2)

RCT J 106-49-0  
SOL 64-19-7 AcOH  
CON 4 hours, reflux

PRO K 22316-59-2

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 66 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

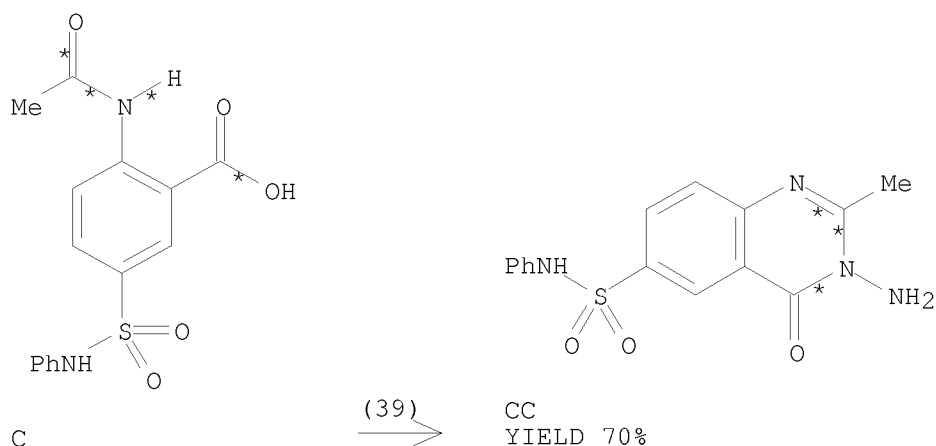
ACCESSION NUMBER: 141:350117 CASREACT

TITLE: Synthesis of 5-arylaminosulpho-N-acetylanthranilic acid, 6-arylaminosulpho-2-methyl-3-amino/3-N-chloroacetamido/3-N-aryl amino

acetamido-4-(3H)-quinazolones as potential anti-HIV,  
anticancer and antimicrobial agents  
AUTHOR(S): Purohit, D. M.; Bhuva, V. R.; Shah, V. H.  
CORPORATE SOURCE: Department of Chemistry, Saurashtra University,  
Rajkot, 360 005, India  
SOURCE: Chemistry (Rajkot, India) (2003), 1(4), 233-245  
CODEN: CHEMCT; ISSN: 0972-8376  
PUBLISHER: Trade Science Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB 5-Arlyminosulfo-N-acetylanthranilic acids,  
3-amino-2-methyl-6-arylaminosulfo-4-(3H)-quinazolone,  
3-N-(chloroacetamido)-2-methyl-6-arylaminosuplho-4-(3H)-quinazolones,  
3-N-(arylinoacetamido)-2-2 methyl-6-arylaminosulfo-4-(3H)-quniazolones  
have been synthesized. The products have been assayed for their anti-HIV  
activity, some of the products showed moderate activity in comparison to  
standard drug AZT. Anticancer activity were tested at five different  
concentration  
against 60 cell lines of human for nine types of cancers. Some of the  
comps. gave less activity as compare to 5-fluorodeoxyuridine (Standard drug).  
The products have been also evaluated for their antimicrobial activity by  
cup - plate method. Some of the comps. showed comparable antimicrobial  
activity with known antibiotics viz. Ampicillin, chloramphenicol,  
Norfloxacin and Griseofulvin. The constitution of the products have been  
delineated by IR, PMR, Mass spectral study and elemental analyses.

RX(39) OF 372 ...C ==> CC...



RX(39) RCT C 774216-86-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

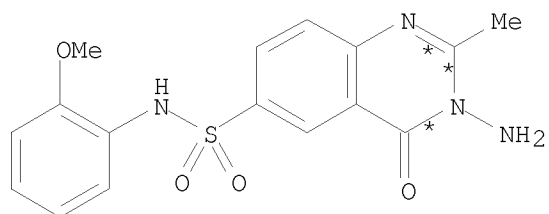
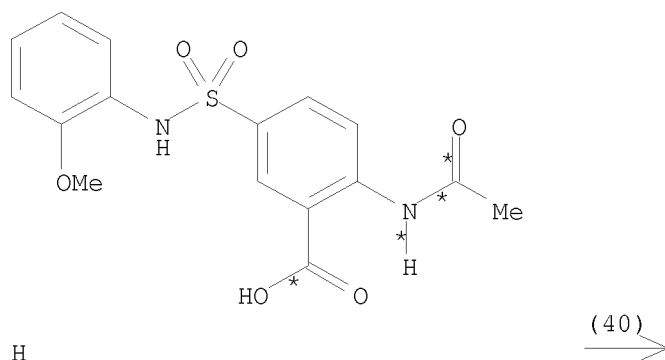
RGT D 7732-18-5 Water  
CON cooled



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PRO CC 774217-23-1  
NTE chemoselective

RX(40) OF 372 ...H ==> CF...



CF  
YIELD 72%

RX(40) RCT H 774216-87-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

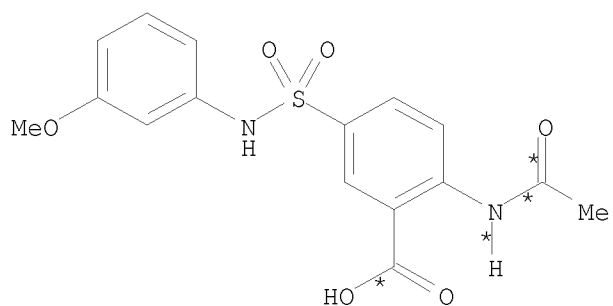
RGT D 7732-18-5 Water

CON cooled

PRO CF 774217-24-2  
NTE chemoselective

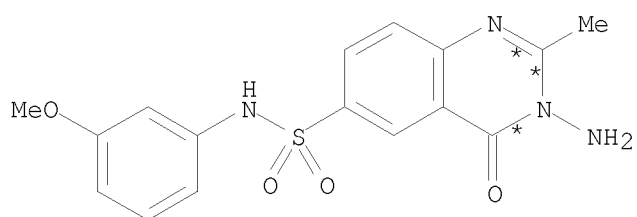
RX(41) OF 372 ...J ==> CG...

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J

(41) 



CG

YIELD 75%

RX(41) RCT J 774216-88-5

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

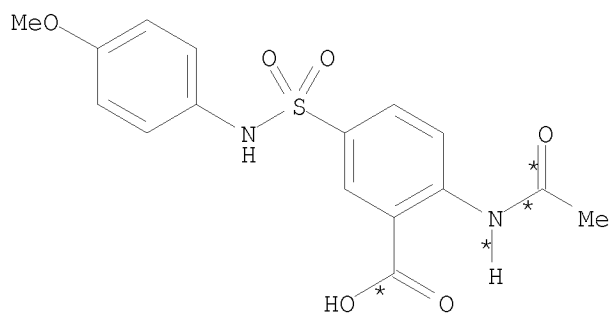
CON cooled

PRO CG 774217-25-3

NTE chemoselective

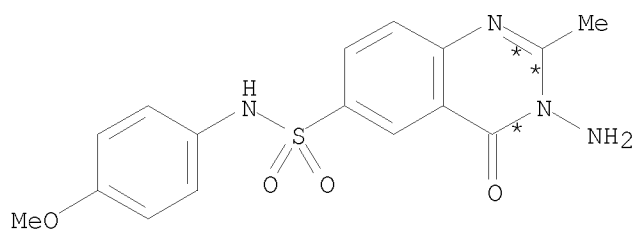
RX(42) OF 372 ...L ==> CH...

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L

(42)



CH

YIELD 73%

RX(42) RCT L 774216-89-6

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

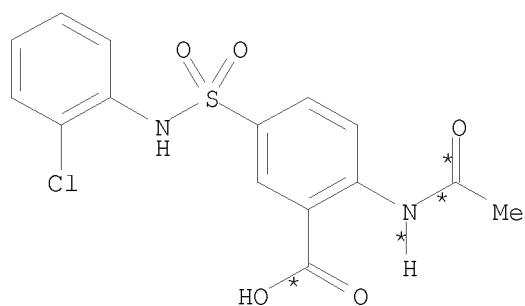
CON cooled

PRO CH 774217-26-4

NTE chemoselective

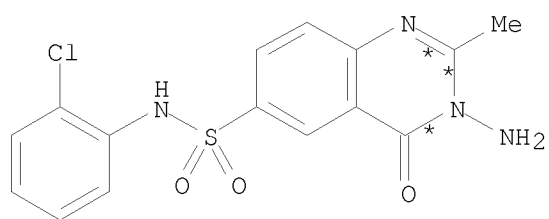
RX(43) OF 372 ...N ==> CI...

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N

(43)  $\longrightarrow$



CI

YIELD 65%

RX(43) RCT N 774216-90-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

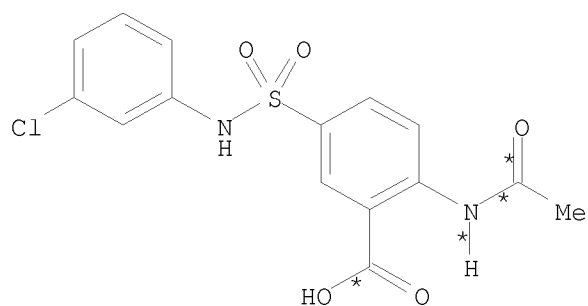
CON cooled

PRO CI 774217-27-5

NTE chemoselective

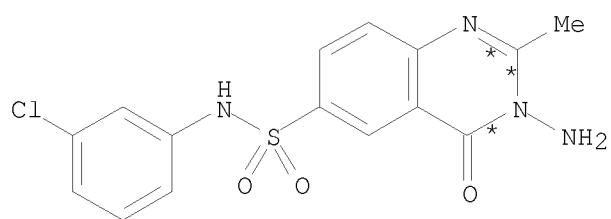
RX(44) OF 372 ...P ==> CJ...

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P

(44)



CJ  
YIELD 68%

RX(44) RCT P 774216-91-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

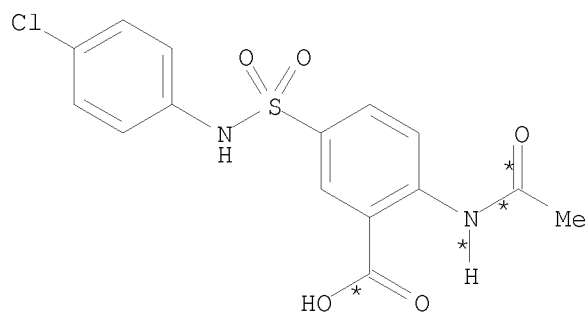
CON cooled

PRO CJ 774217-28-6

NTE chemoselective

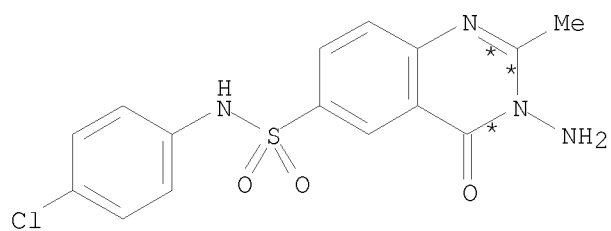
RX(45) OF 372 ...R ==> CK...

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R

(45)  $\longrightarrow$



CK

YIELD 68%

RX(45) RCT R 774216-92-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

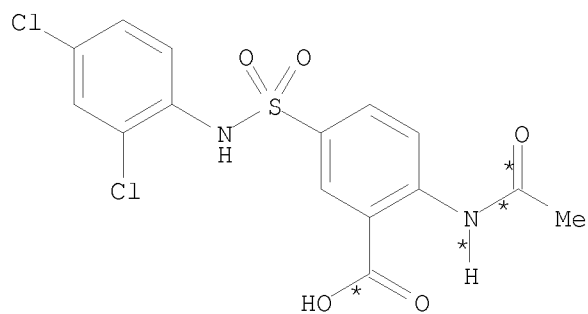
CON cooled

PRO CK 774217-29-7

NTE chemoselective

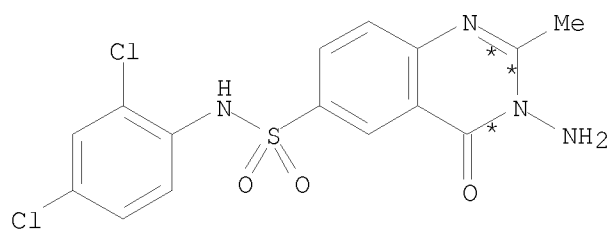
RX(46) OF 372 ...T ==> CL...

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T

(46)  $\longrightarrow$



CL  
YIELD 72%

RX(46) RCT T 774216-93-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

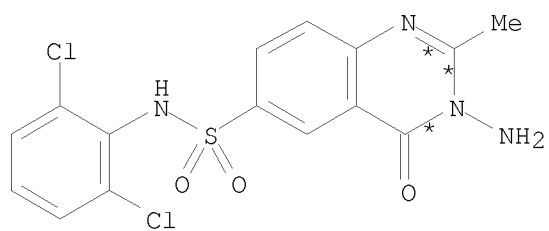
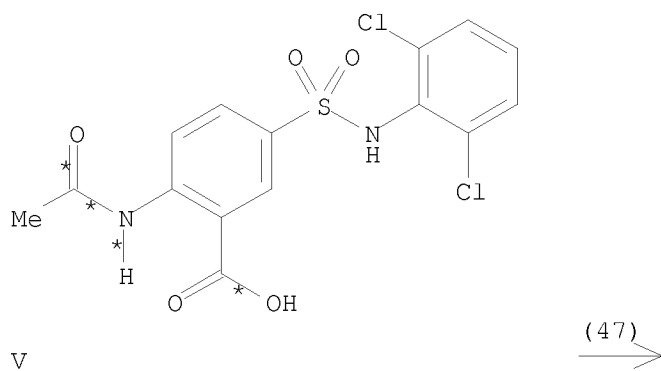
CON cooled

PRO CL 774217-30-0

NTE chemoselective

RX(47) OF 372 ...V ==> CM...

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CM  
YIELD 68%

RX(47) RCT V 774216-94-3

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

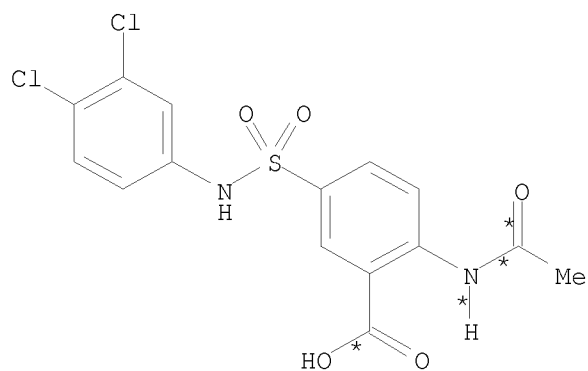
RGT D 7732-18-5 Water  
CON cooled

PRO CM 774217-31-1  
NTE chemoselective

RX(48) OF 372 ...X ==> CN...

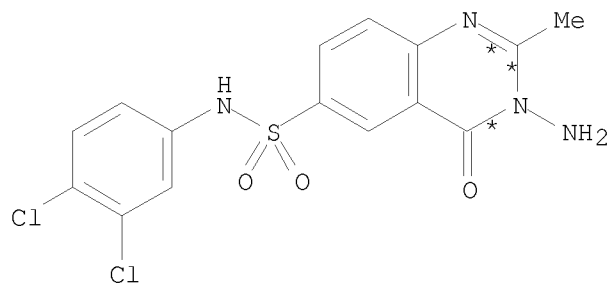


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X

(48)



CN  
YIELD 72%

RX(48) RCT X 774216-95-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

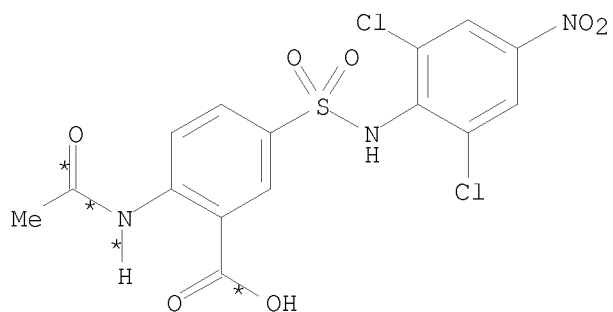
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CN 774217-32-2  
NTE chemoselective

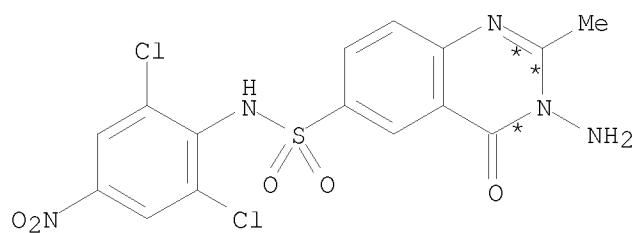
RX(49) OF 372 ...Z ==> CO...

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Z

(49)  $\longrightarrow$



CO

YIELD 81%

RX(49) RCT Z 218617-81-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

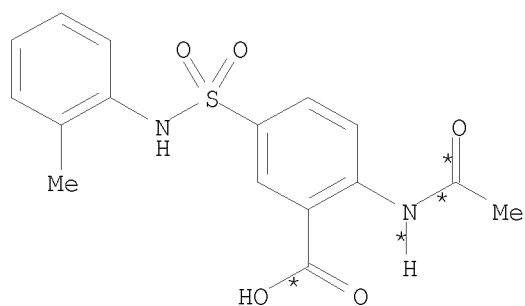
CON cooled

PRO CO 234096-58-3

NTE chemoselective

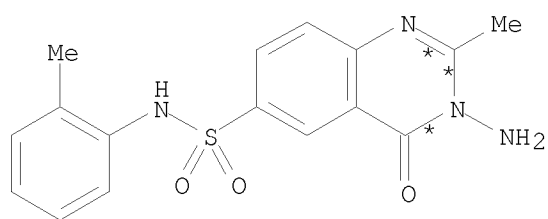
RX(50) OF 372 ...AB ==> CP...

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AB

(50)  $\longrightarrow$



CP

YIELD 72%

RX(50) RCT AB 774216-96-5

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

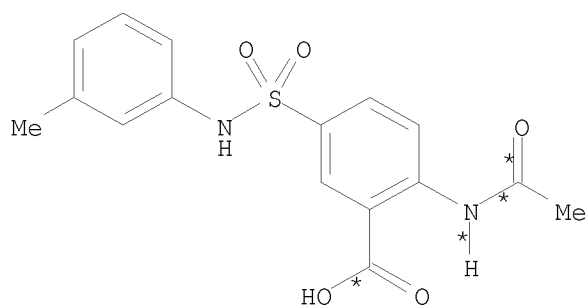
CON cooled

PRO CP 774217-33-3

NTE chemoselective

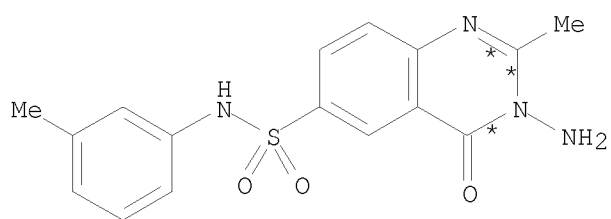
RX(51) OF 372 ...AD ==> CQ...

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AD

(51)



CQ  
YIELD 74%

RX(51) RCT AD 774216-97-6

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

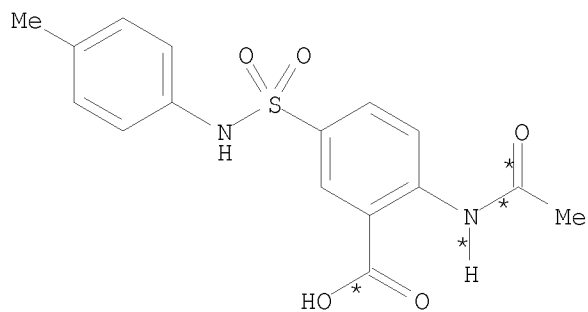
CON cooled

PRO CQ 774217-34-4

NTE chemoselective

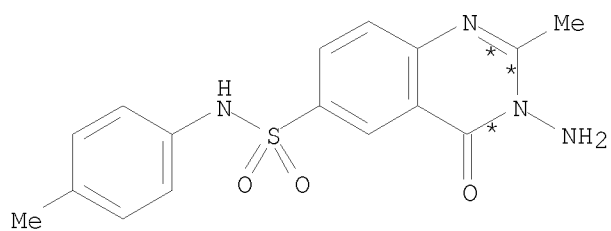
RX(52) OF 372 ...AF ==> CR...

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AF

(52) →



CR  
YIELD 70%

RX(52) RCT AF 774216-98-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

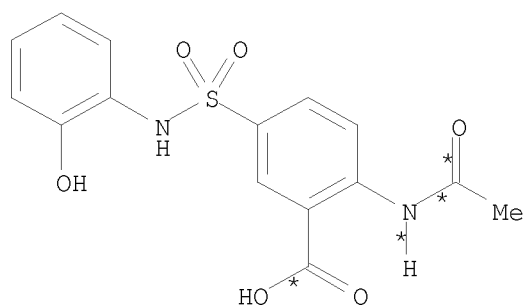
CON cooled

PRO CR 774217-35-5

NTE chemoselective

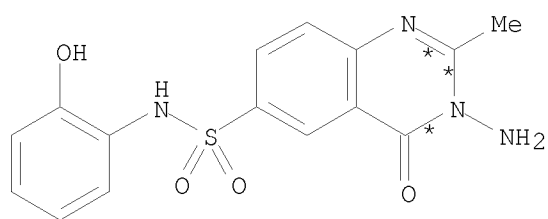
RX(53) OF 372 ...AH ==> CS...

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AH

(53) 



CS

YIELD 76%

RX(53) RCT AH 774216-99-8

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

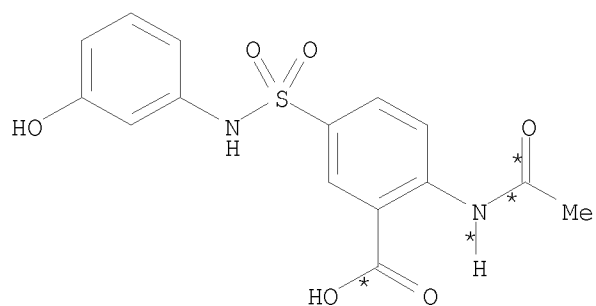
CON cooled

PRO CS 774217-36-6

NTE chemoselective

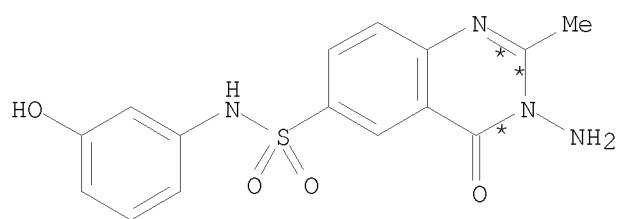
RX(54) OF 372 ...AJ ==> CT...

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AJ

(54)  $\longrightarrow$



CT

YIELD 76%

RX(54) RCT AJ 774217-00-4

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

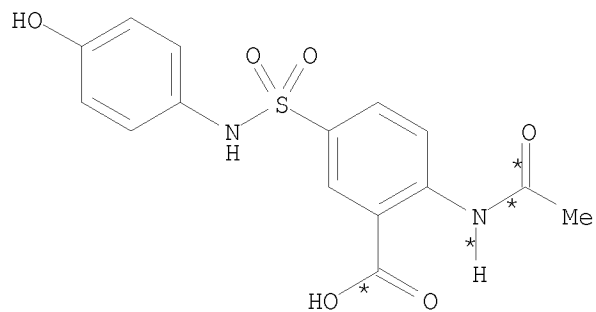
CON cooled

PRO CT 774217-37-7

NTE chemoselective

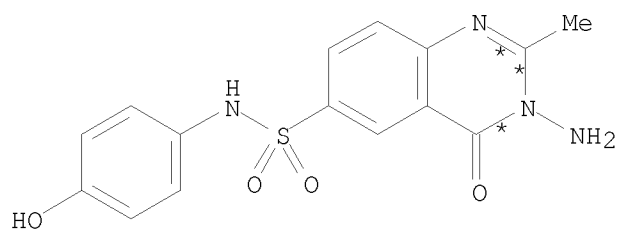
RX(55) OF 372 ...AL ==> CU...

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AL

(55) →



CU

YIELD 72%

RX(55) RCT AL 774217-01-5

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

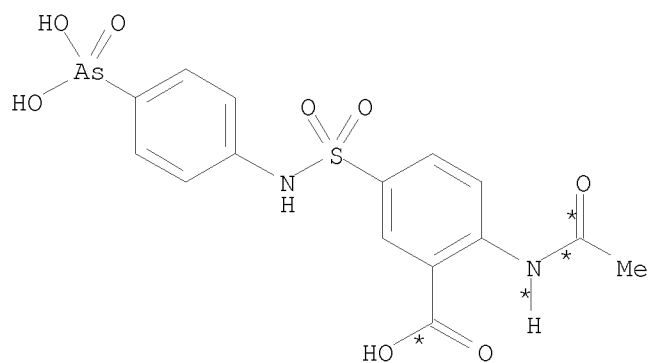
PRO CU 774217-38-8

NTE chemoselective

RX(56) OF 372 ...AN ==> CV...

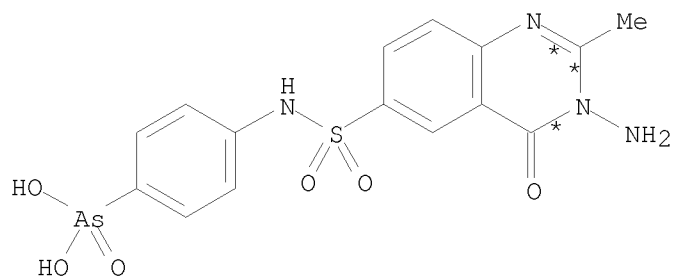


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AN

(56)



CV  
YIELD 81%

RX(56)      RCT    AN 774217-02-6

STAGE(1)

RGT    CD 7803-57-8 N2H4-H2O  
SOL    67-56-1 MeOH  
CON    3 hours, reflux

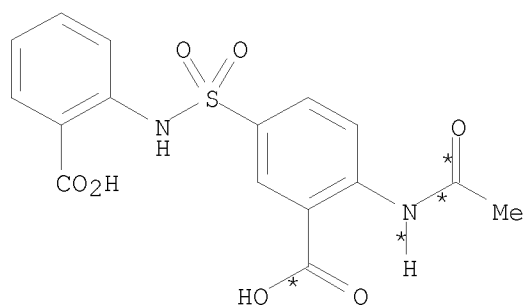
STAGE(2)

RGT    D 7732-18-5 Water  
CON    cooled

PRO    CV 774217-39-9  
NTE    chemoselective

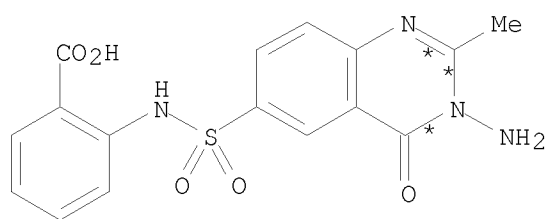
RX(57) OF 372      ...AP ==> CW...

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AP

(57)  $\longrightarrow$



CW

YIELD 81%

RX(57) RCT AP 774217-03-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

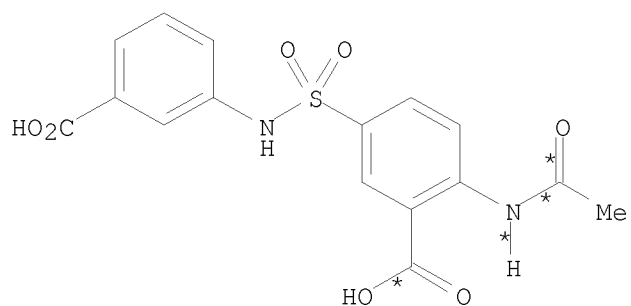
CON cooled

PRO CW 774217-40-2

NTE chemoselective

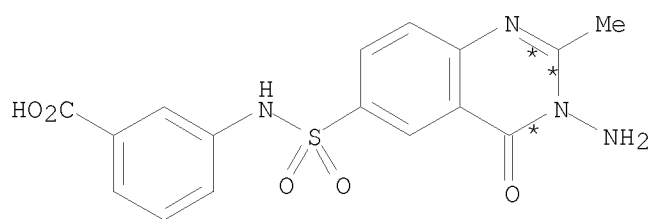
RX(58) OF 372 ...AR ==> CX...

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AR

(58)  $\longrightarrow$



CX

YIELD 82%

RX(58) RCT AR 774217-04-8

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

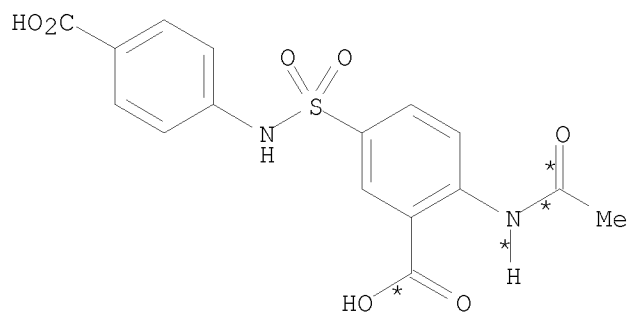
CON cooled

PRO CX 774217-41-3

NTE chemoselective

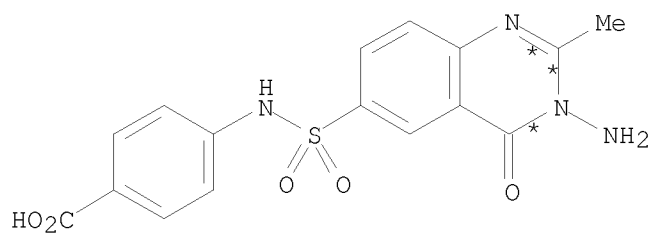
RX(59) OF 372 ...AT ==> CY...

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AT

(59)  $\longrightarrow$



CY

YIELD 81%

RX(59) RCT AT 774217-05-9

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

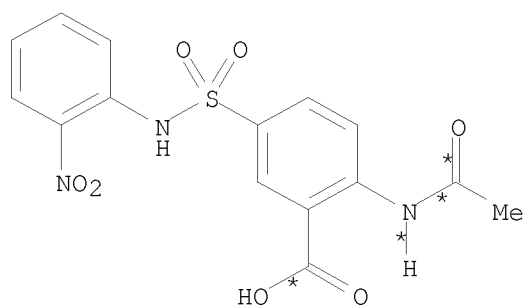
CON cooled

PRO CY 774217-42-4

NTE chemoselective

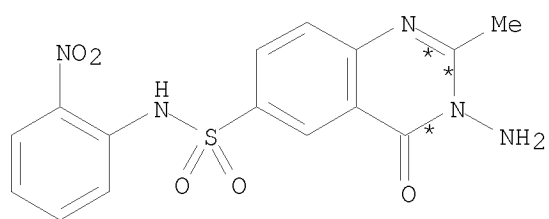
RX(60) OF 372 ...AV ==> CZ...

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AV

(60)  $\longrightarrow$



CZ

YIELD 78%

RX(60) RCT AV 774217-06-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

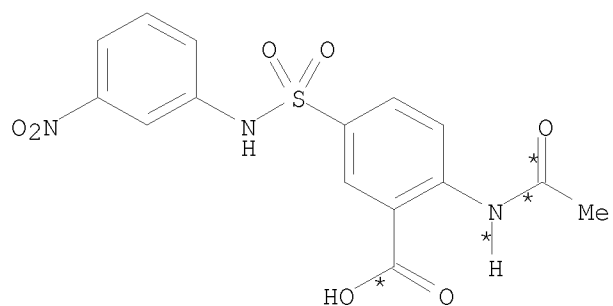
CON cooled

PRO CZ 774217-43-5

NTE chemoselective

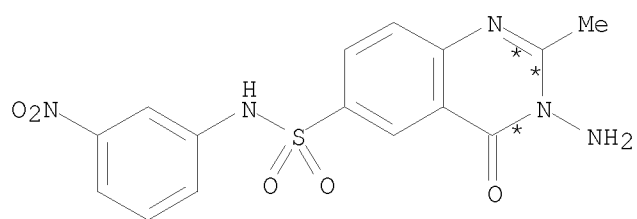
RX(61) OF 372 ...AX ==> DA...

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AX

(61)  $\longrightarrow$



DA

YIELD 76%

RX(61) RCT AX 774217-07-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

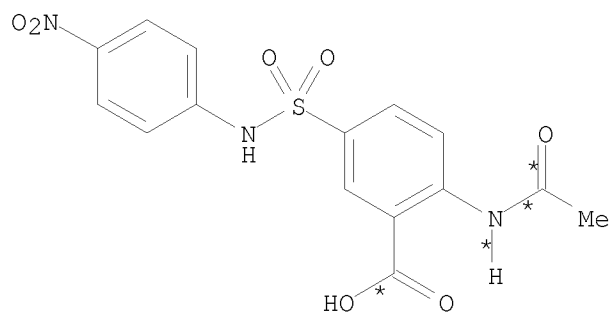
CON cooled

PRO DA 774217-44-6

NTE chemoselective

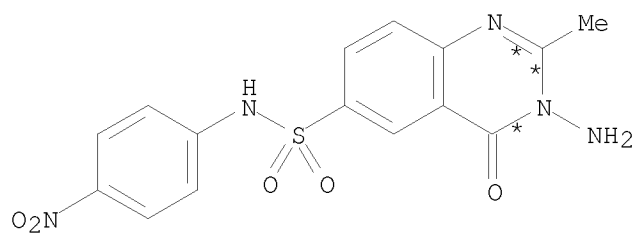
RX(62) OF 372 ...AZ ==> DB...

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AZ

(62)  $\longrightarrow$



DB

YIELD 79%

RX(62) RCT AZ 774217-08-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

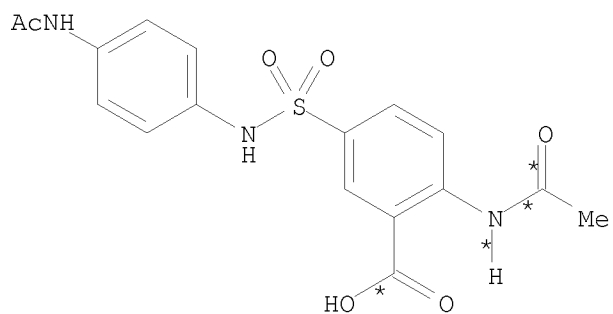
CON cooled

PRO DB 774217-45-7

NTE chemoselective

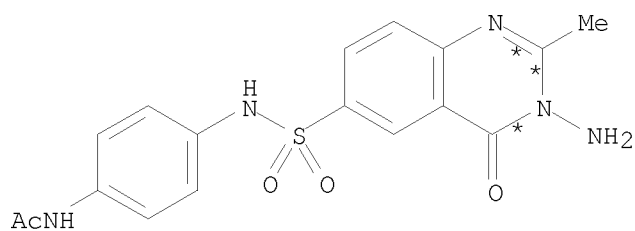
RX(63) OF 372 ...BB ==> DC...

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BB

(63)  $\longrightarrow$



DC

YIELD 71%

RX(63) RCT BB 774217-09-3

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

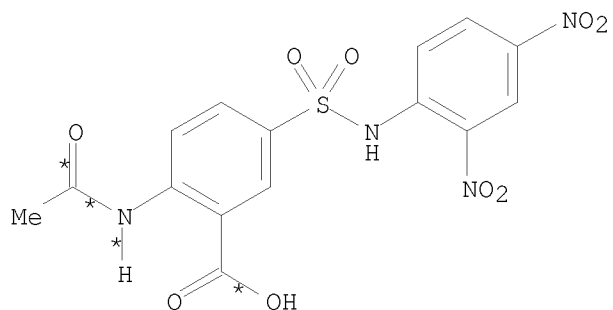
PRO DC 774217-46-8

NTE chemoselective

RX(64) OF 372 ...BD ==> DD...

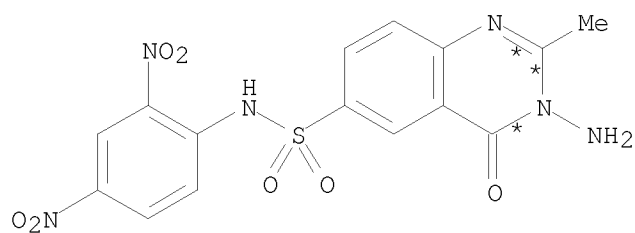


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BD

(64)  $\longrightarrow$



DD

YIELD 76%

RX(64) RCT BD 774217-10-6

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

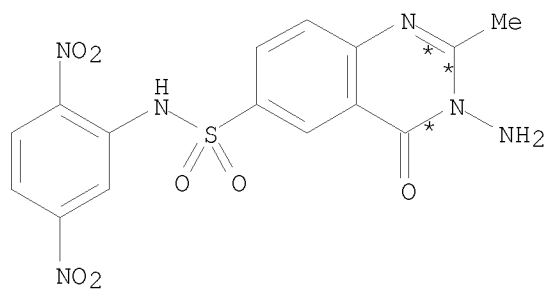
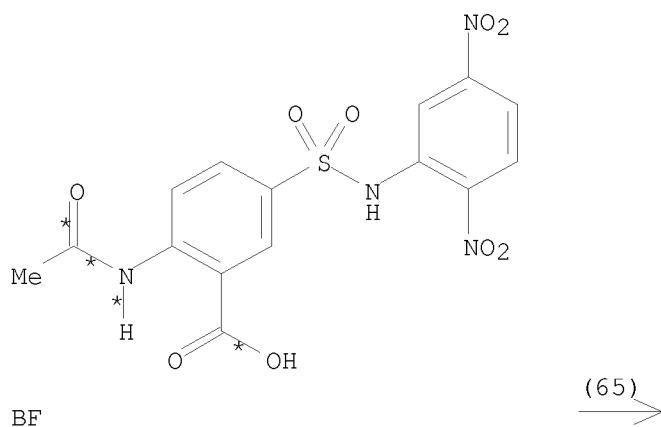
CON cooled

PRO DD 774217-47-9

NTE chemoselective

RX(65) OF 372 ...BF ==> DE...

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DE  
YIELD 78%

RX(65) RCT BF 774217-11-7

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

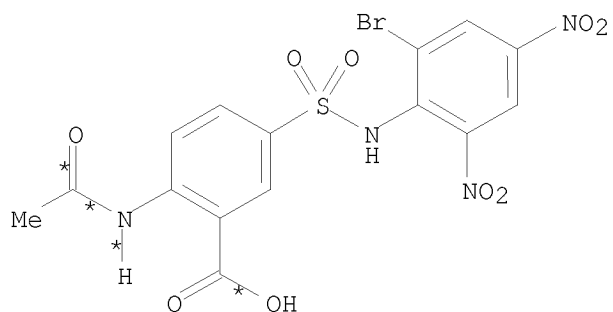
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DE 774217-48-0  
NTE chemoselective

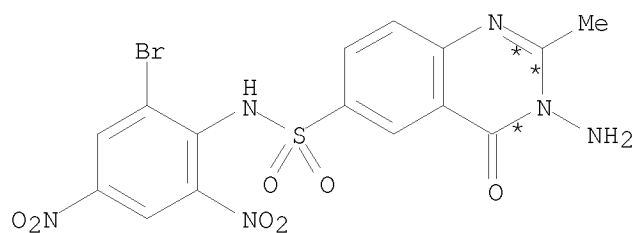
RX(66) OF 372 ...BH ==> DF...

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BH

(66)  $\longrightarrow$



DF

YIELD 72%

RX(66) RCT BH 774217-12-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

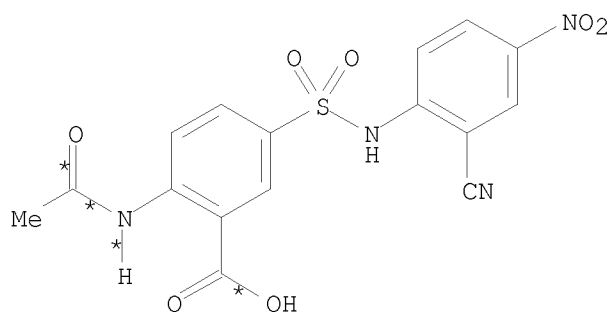
CON cooled

PRO DF 774217-49-1

NTE chemoselective

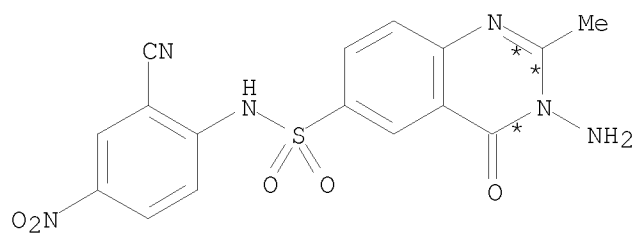
RX(67) OF 372 ...BJ ==> DG...

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BJ

(67)  $\longrightarrow$



DG

YIELD 71%

RX(67) RCT BJ 774217-13-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

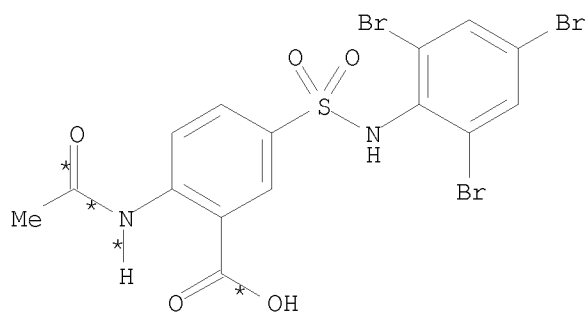
CON cooled

PRO DG 774217-50-4

NTE chemoselective

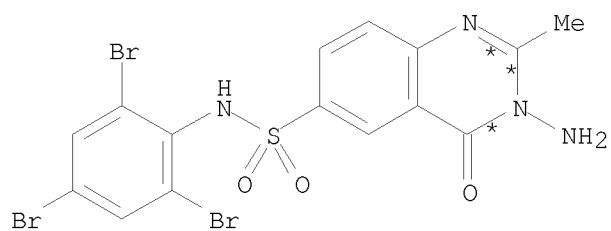
RX(68) OF 372 ...BL ==> DH...

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BL

(68)  $\longrightarrow$



DH

YIELD 80%

RX(68) RCT BL 774217-14-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

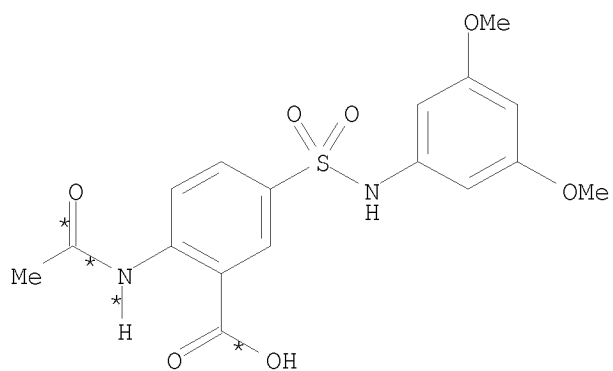
CON cooled

PRO DH 774217-51-5

NTE chemoselective

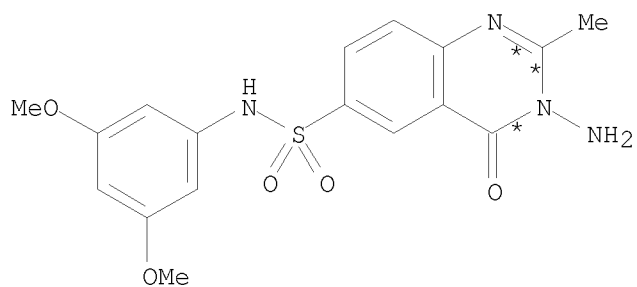
RX(69) OF 372 ...BN ==> DI...

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BN

(69)



DI  
YIELD 75%

RX(69) RCT BN 774217-15-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

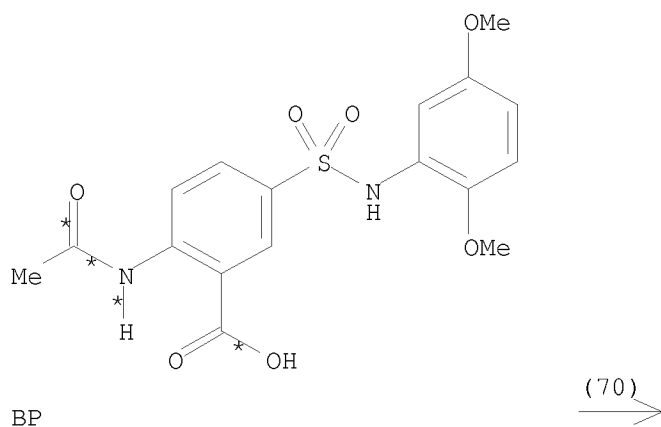
CON cooled

PRO DI 774217-52-6

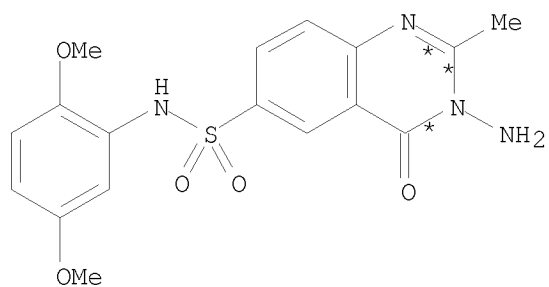
NTE chemoselective

RX(70) OF 372 ...BP ==> DJ...

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BP



DJ  
YIELD 72%

RX(70) RCT BP 774217-16-2

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

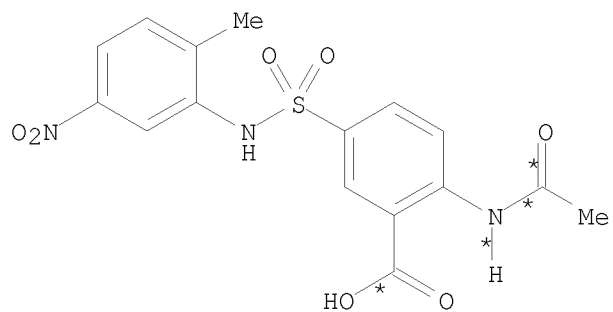
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DJ 774217-53-7  
NTE chemoselective

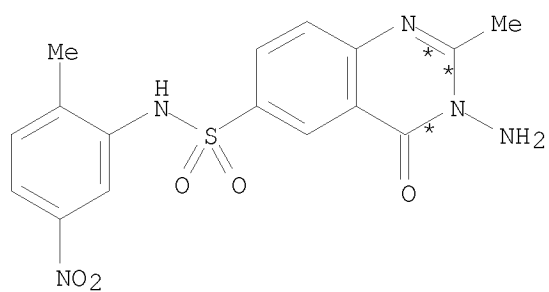
RX(71) OF 372 ...BR ==> DK...

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BR

(71)  $\longrightarrow$



DK

YIELD 68%

RX(71) RCT BR 774217-17-3

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

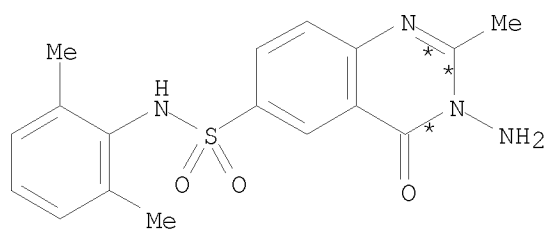
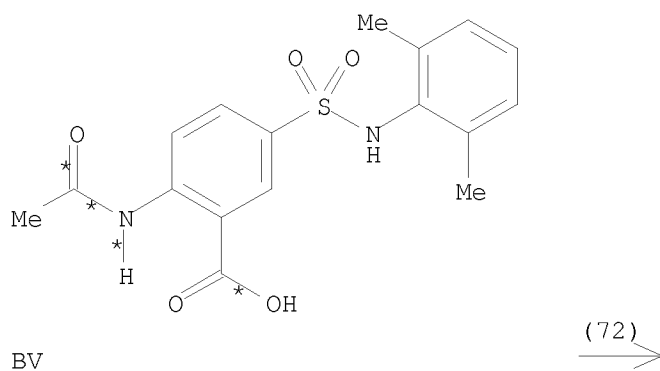
PRO DK 774217-54-8

NTE chemoselective

RX(72) OF 372 ...BV ==> DL...



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DL  
YIELD 72%

RX(72) RCT BV 774217-19-5

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

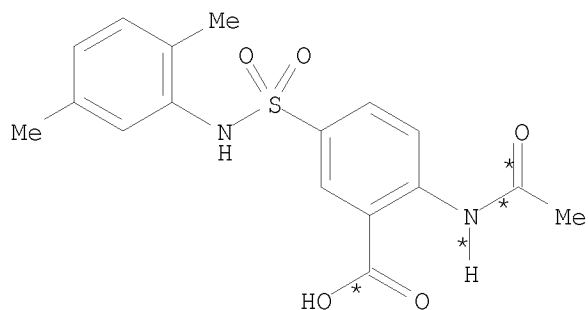
CON cooled

PRO DL 774217-56-0

NTE chemoselective

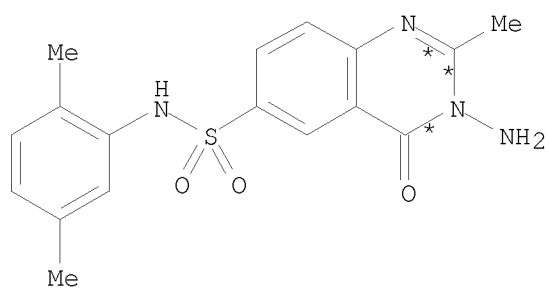
RX(73) OF 372 ...BX ==> DM...

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BX

(73) →



DM

YIELD 70%

RX(73) RCT BX 774217-20-8

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

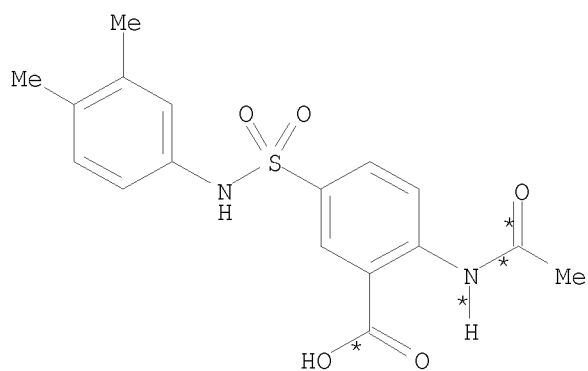
CON cooled

PRO DM 774217-57-1

NTE chemoselective

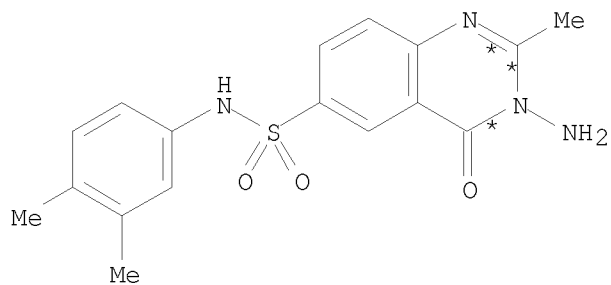
RX(74) OF 372 ...BZ ==> DN...

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BZ

(74)



DN  
YIELD 75%

RX(74) RCT BZ 774217-21-9

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

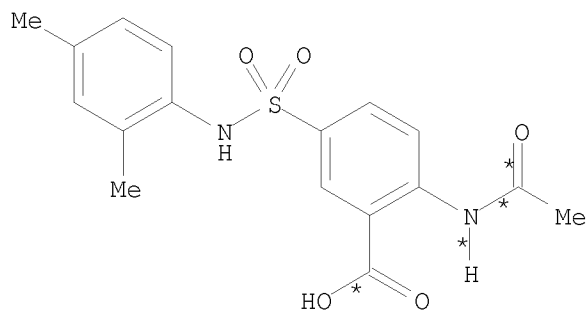
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DN 774217-58-2  
NTE chemoselective

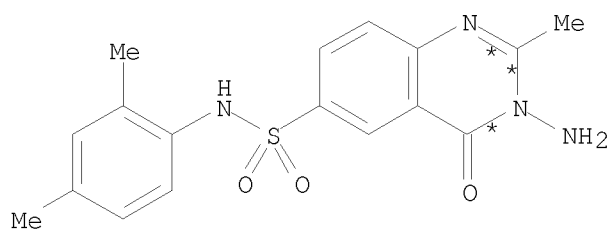
RX(75) OF 372 ...CB ==> DO...

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CB

(75)  $\longrightarrow$



DO  
YIELD 77%

RX(75) RCT CB 774217-22-0

STAGE(1)

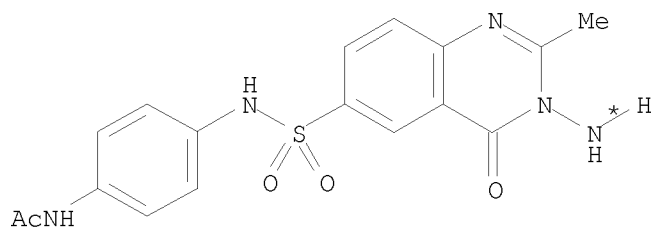
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

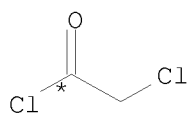
RGT D 7732-18-5 Water  
CON cooled

PRO DO 774217-59-3  
NTE chemoselective

RX(100) OF 372 ...DC + DP ==> EO...



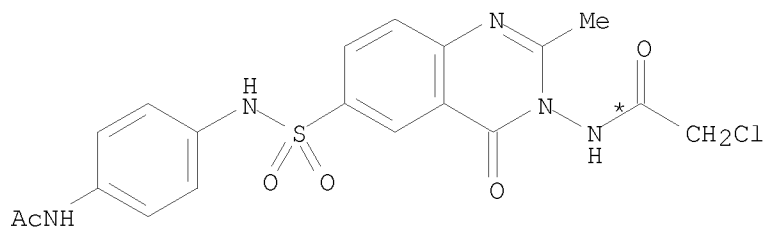
DC



DP

(100)  $\longrightarrow$

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EO  
YIELD 53%

RX(100) RCT DC 774217-46-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

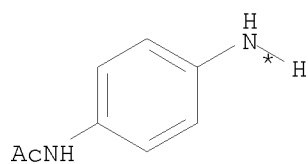
STAGE(2)

RGT D 7732-18-5 Water

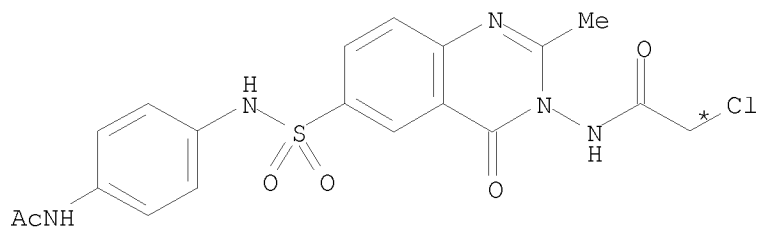
CON cooled

PRO EO 774217-84-4

RX(137) OF 372 ...BA + EO ==> FZ



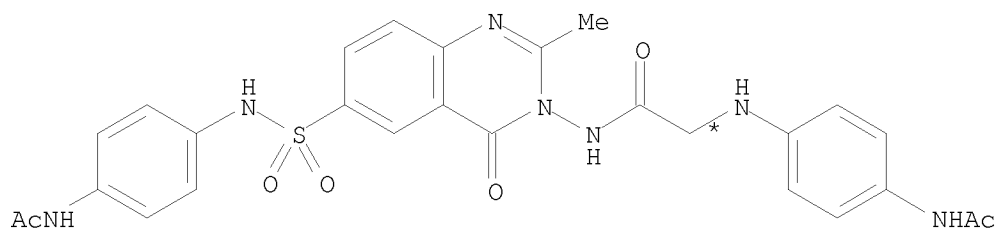
BA



EO

(137)  
→

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FZ  
YIELD 53%

RX(137) RCT BA 122-80-5, EO 774217-84-4

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

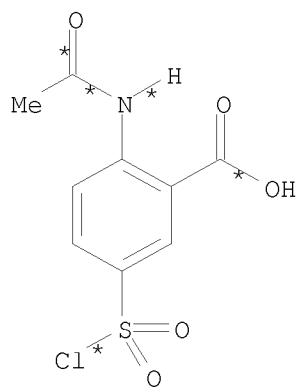
RGT D 7732-18-5 Water

CON cooled

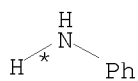
PRO FZ 774218-18-7

RX(151) OF 372 COMPOSED OF RX(1), RX(39)

RX(151) A + B ==> CC



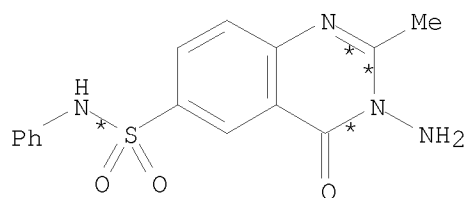
A



B

2  
STEPS  
→

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CC  
YIELD 70%

RX(1) RCT A 181478-44-4, B 62-53-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO C 774216-86-3

RX(39) RCT C 774216-86-3

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

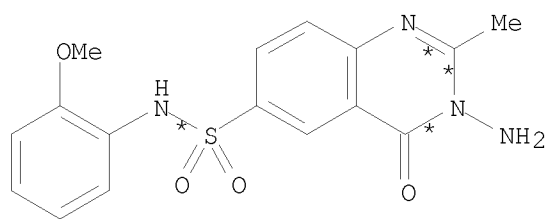
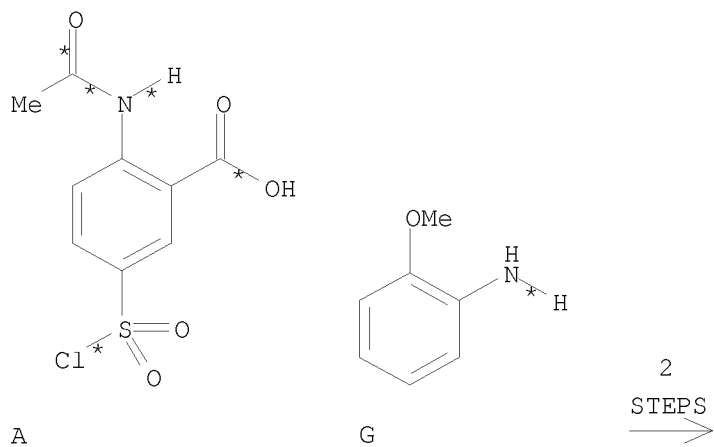
PRO CC 774217-23-1

NTE chemoselective

RX(152) OF 372 COMPOSED OF RX(2), RX(40)

RX(152) A + G ==> CF

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CF  
YIELD 72%

RX(2) RCT A 181478-44-4, G 90-04-0

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO H 774216-87-4

RX(40) RCT H 774216-87-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

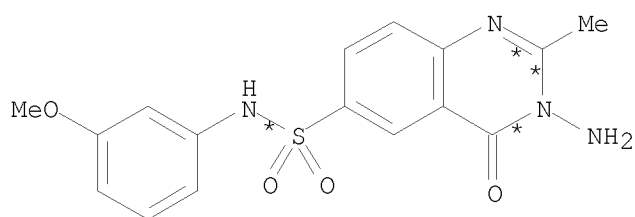
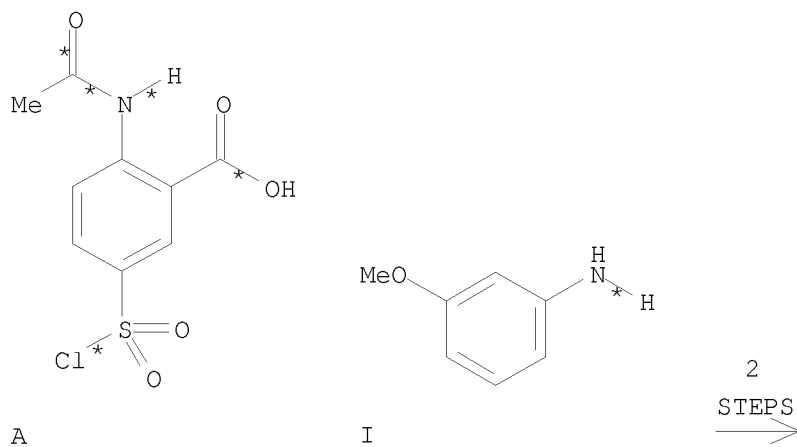
CON cooled



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PRO CF 774217-24-2  
NTE chemoselective

RX(153) OF 372 COMPOSED OF RX(3), RX(41)  
RX(153) A + I ==> CG



CG  
YIELD 75%

RX(3) RCT A 181478-44-4, I 536-90-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO J 774216-88-5

RX(41) RCT J 774216-88-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

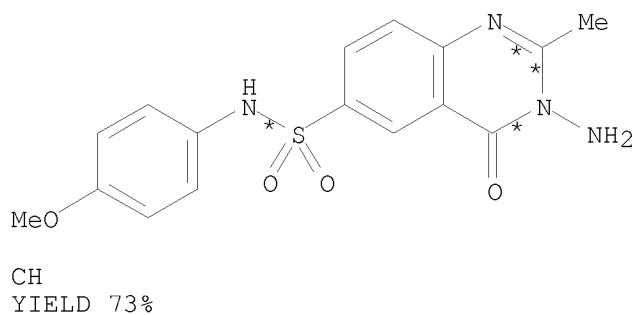
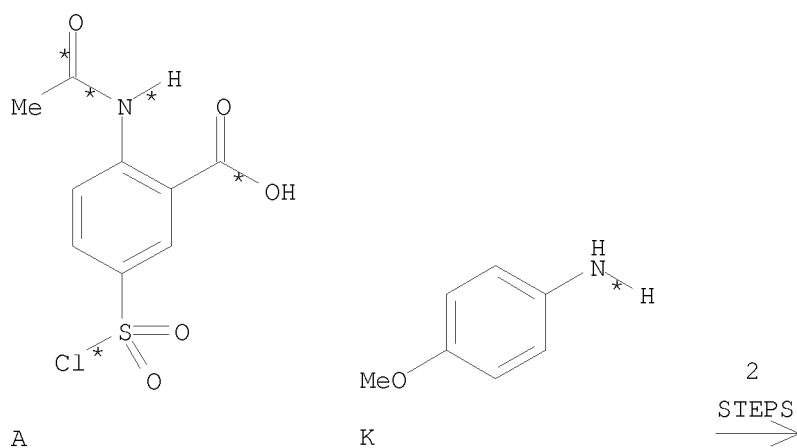
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SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CG 774217-25-3  
NTE chemoselective

RX(154) OF 372 COMPOSED OF RX(4), RX(42)  
RX(154) A + K ==> CH



RX(4) RCT A 181478-44-4, K 104-94-9

STAGE(1)  
CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

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PRO L 774216-89-6

RX(42) RCT L 774216-89-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

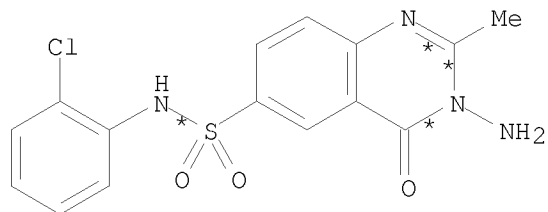
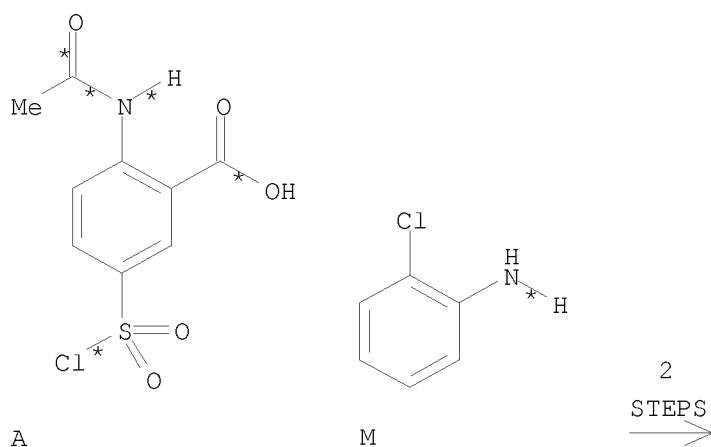
CON cooled

PRO CH 774217-26-4

NTE chemoselective

RX(155) OF 372 COMPOSED OF RX(5), RX(43)

RX(155) A + M ==> CI



CI  
YIELD 65%

RX(5) RCT A 181478-44-4, M 95-51-2

STAGE(1)

CAT 110-86-1 Pyridine

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SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO N 774216-90-9

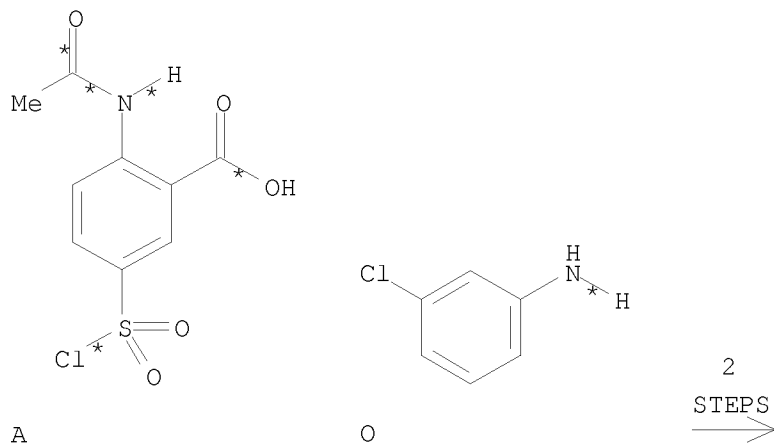
RX(43) RCT N 774216-90-9

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

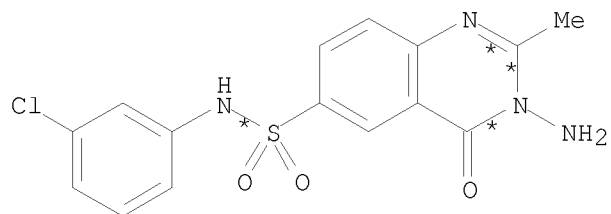
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CI 774217-27-5  
NTE chemoselective

RX(156) OF 372 COMPOSED OF RX(6), RX(44)  
RX(156) A + O ==> CJ



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CJ  
YIELD 68%

RX(6) RCT A 181478-44-4, O 108-42-9

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO P 774216-91-0

RX(44) RCT P 774216-91-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

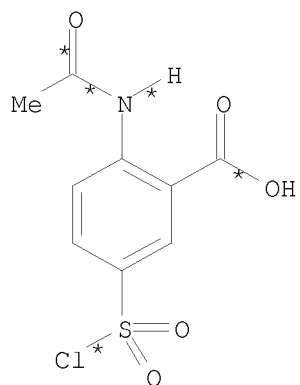
PRO CJ 774217-28-6

NTE chemoselective

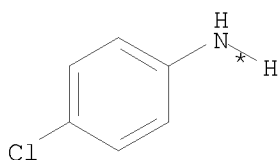
RX(157) OF 372 COMPOSED OF RX(7), RX(45)

RX(157) A + Q ==> CK

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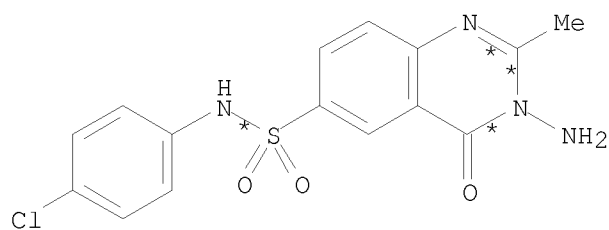


A



Q

2  
STEPS  
→



CK  
YIELD 68%

RX(7) RCT A 181478-44-4, Q 106-47-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO R 774216-92-1

RX(45) RCT R 774216-92-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

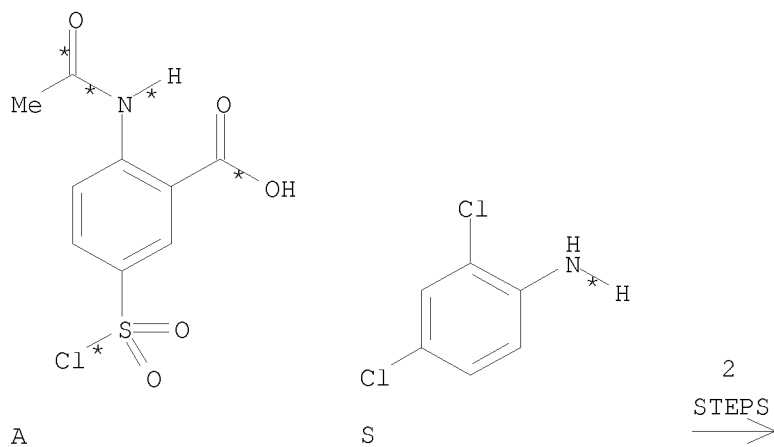
RGT D 7732-18-5 Water

CON cooled

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PRO CK 774217-29-7  
NTE chemoselective

RX(158) OF 372 COMPOSED OF RX(8), RX(46)  
RX(158) A + S ==> CL



CL  
YIELD 72%

RX(8) RCT A 181478-44-4, S 554-00-7

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO T 774216-93-2

RX(46) RCT T 774216-93-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

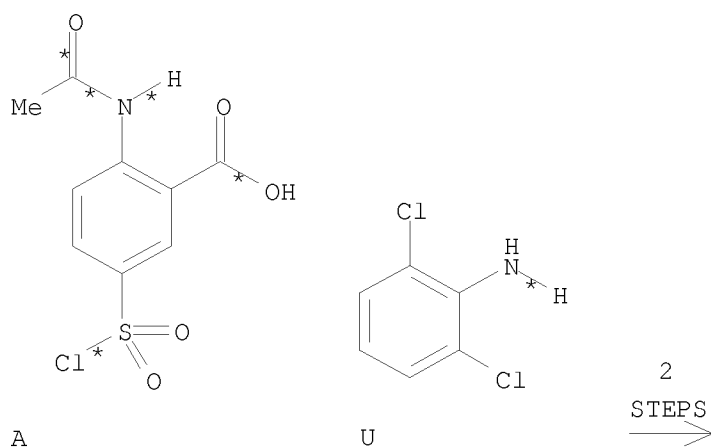
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SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CL 774217-30-0  
NTE chemoselective

RX(159) OF 372 COMPOSED OF RX(9), RX(47)  
RX(159) A + U ==> CM



CM  
YIELD 68%

RX(9) RCT A 181478-44-4, U 608-31-1

STAGE(1)  
CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled



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PRO V 774216-94-3

RX(47) RCT V 774216-94-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

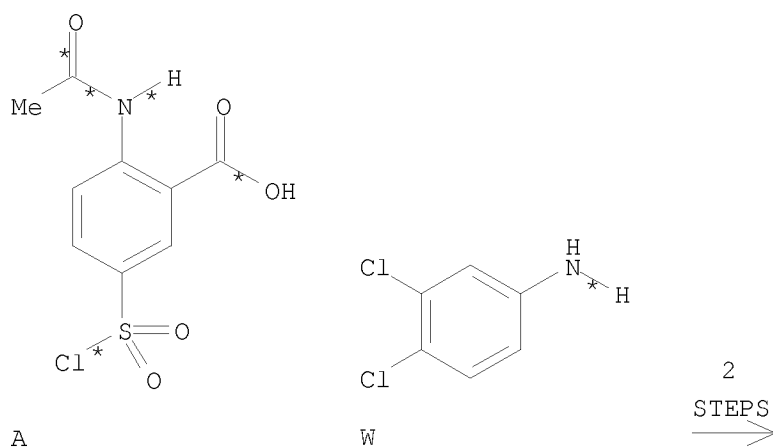
CON cooled

PRO CM 774217-31-1

NTE chemoselective

RX(160) OF 372 COMPOSED OF RX(10), RX(48)

RX(160) A + W ==> CN



CN  
YIELD 72%

RX(10) RCT A 181478-44-4, W 95-76-1

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STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO X 774216-95-4

RX(48) RCT X 774216-95-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

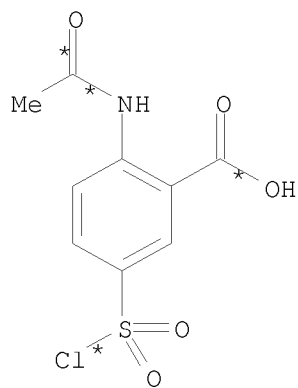
CON cooled

PRO CN 774217-32-2

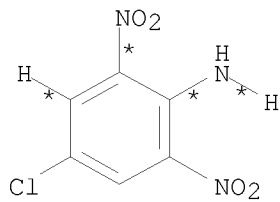
NTE chemoselective

RX(161) OF 372 COMPOSED OF RX(11), RX(49)

RX(161) A + Y ==> CO



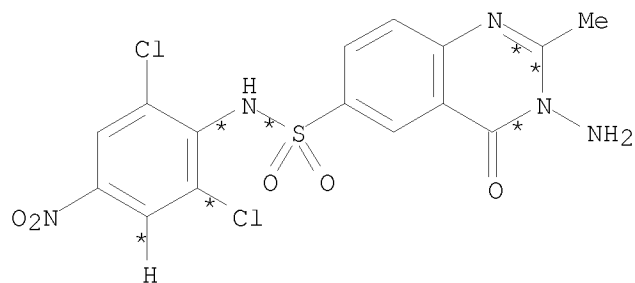
A



Y

2  
STEPS  
→

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CO  
YIELD 81%

RX(11) RCT A 181478-44-4, Y 5388-62-5

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO Z 218617-81-3

RX(49) RCT Z 218617-81-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

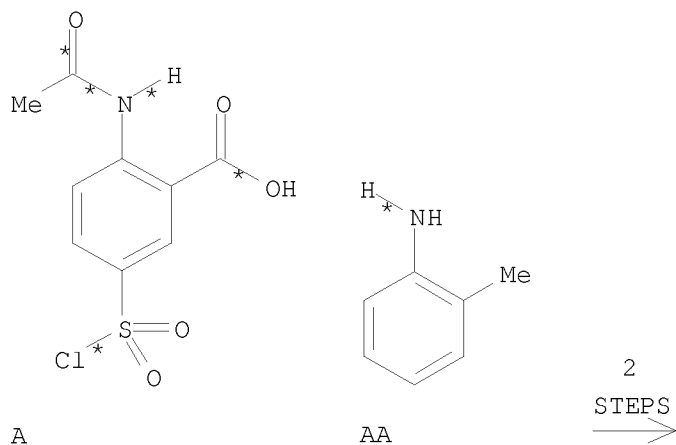
PRO CO 234096-58-3

NTE chemoselective

RX(162) OF 372 COMPOSED OF RX(12), RX(50)

RX(162) A + AA ==> CP

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CP  
YIELD 72%

RX(12) RCT A 181478-44-4, AA 95-53-4

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AB 774216-96-5

RX(50) RCT AB 774216-96-5

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

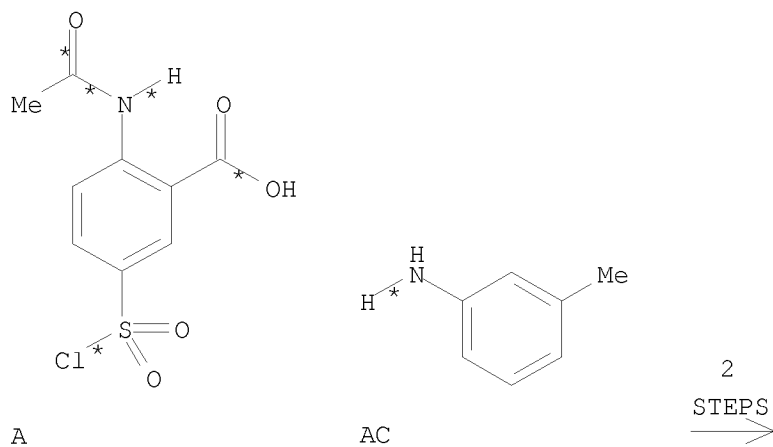
RGT D 7732-18-5 Water

CON cooled

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PRO CP 774217-33-3  
NTE chemoselective

RX(163) OF 372 COMPOSED OF RX(13), RX(51)  
RX(163) A + AC ==> CQ



CQ  
YIELD 74%

RX(13) RCT A 181478-44-4, AC 108-44-1

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AD 774216-97-6

RX(51) RCT AD 774216-97-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

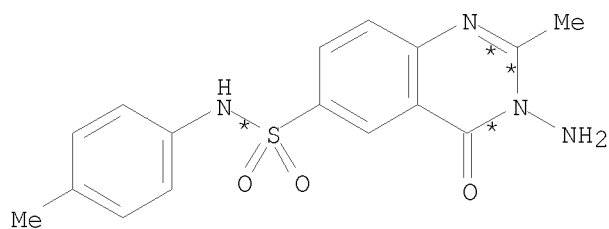
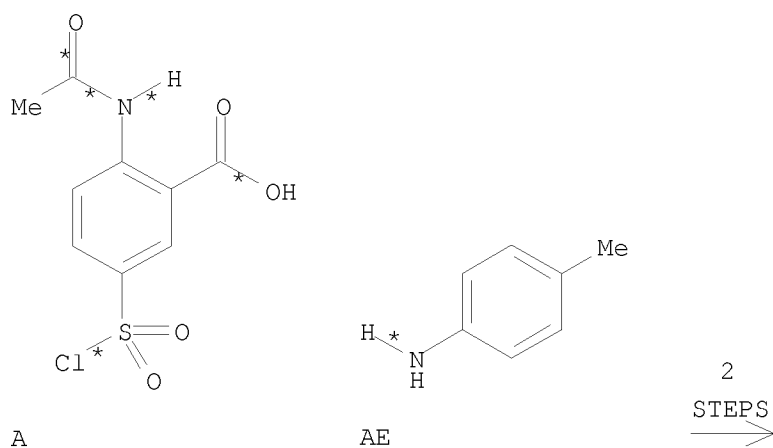
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SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CQ 774217-34-4  
NTE chemoselective

RX(164) OF 372 COMPOSED OF RX(14), RX(52)  
RX(164) A + AE ==> CR



CR  
YIELD 70%

RX(14) RCT A 181478-44-4, AE 106-49-0

STAGE(1)  
CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

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PRO AF 774216-98-7

RX(52) RCT AF 774216-98-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

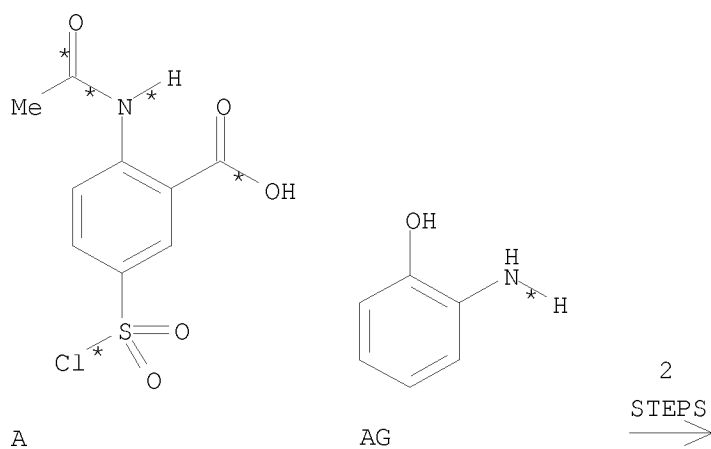
CON cooled

PRO CR 774217-35-5

NTE chemoselective

RX(165) OF 372 COMPOSED OF RX(15), RX(53)

RX(165) A + AG ==> CS



CS  
YIELD 76%

RX(15) RCT A 181478-44-4, AG 95-55-6

STAGE(1)

CAT 110-86-1 Pyridine

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SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO AH 774216-99-8

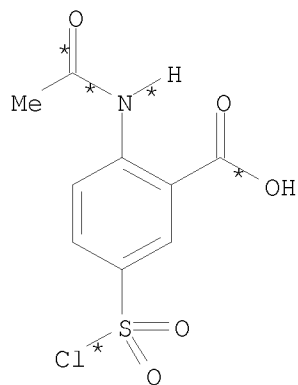
RX(53) RCT AH 774216-99-8

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

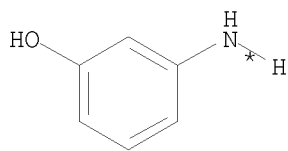
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CS 774217-36-6  
NTE chemoselective

RX(166) OF 372 COMPOSED OF RX(16), RX(54)  
RX(166) A + AI ==> CT



A

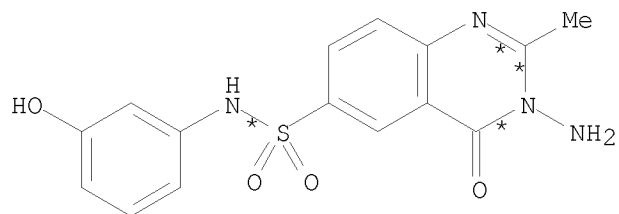


AI

2  
STEPS  
→



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CT  
YIELD 76%

RX(16) RCT A 181478-44-4, AI 591-27-5

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AJ 774217-00-4

RX(54) RCT AJ 774217-00-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

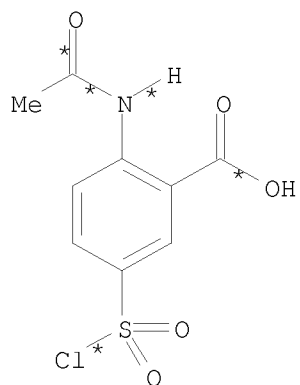
PRO CT 774217-37-7

NTE chemoselective

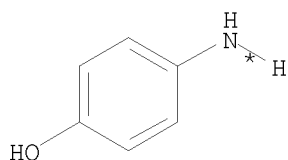
RX(167) OF 372 COMPOSED OF RX(17), RX(55)

RX(167) A + AK ==> CU

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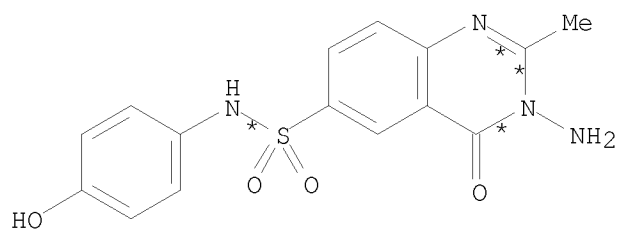


A



AK

2  
STEPS  
→



CU

YIELD 72%

RX(17) RCT A 181478-44-4, AK 123-30-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AL 774217-01-5

RX(55) RCT AL 774217-01-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

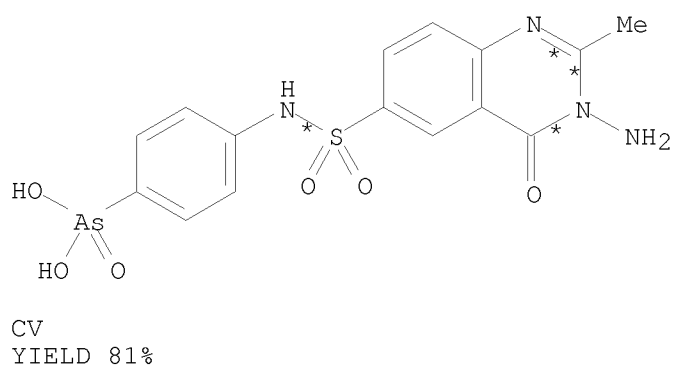
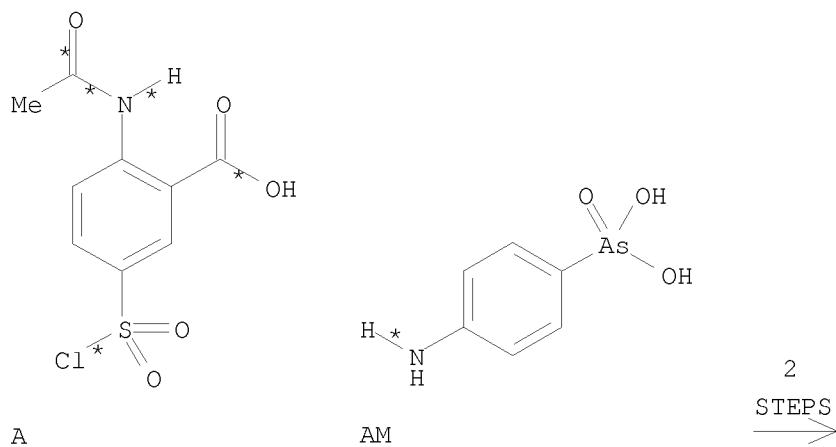
RGT D 7732-18-5 Water

CON cooled

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PRO CU 774217-38-8  
NTE chemoselective

RX(168) OF 372 COMPOSED OF RX(18), RX(56)  
RX(168) A + AM ==> CV



RX(18) RCT A 181478-44-4, AM 98-50-0

STAGE(1)

CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO AN 774217-02-6

RX(56) RCT AN 774217-02-6

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STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

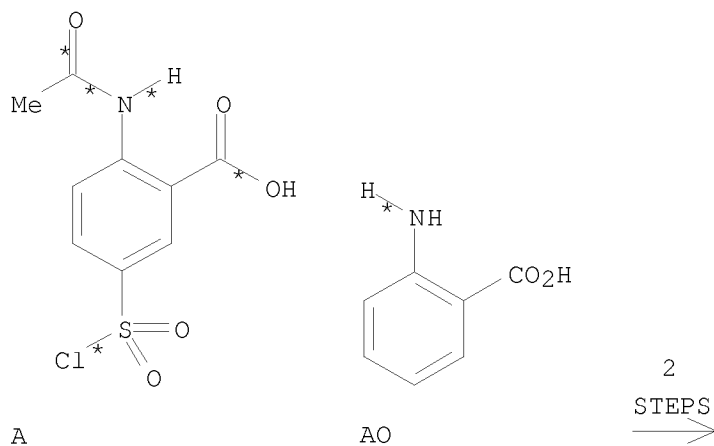
CON cooled

PRO CV 774217-39-9

NTE chemoselective

RX(169) OF 372 COMPOSED OF RX(19), RX(57)

RX(169) A + AO ==> CW



CW  
YIELD 81%

RX(19) RCT A 181478-44-4, AO 118-92-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

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RGT D 7732-18-5 Water  
CON cooled

PRO AP 774217-03-7

RX(57) RCT AP 774217-03-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

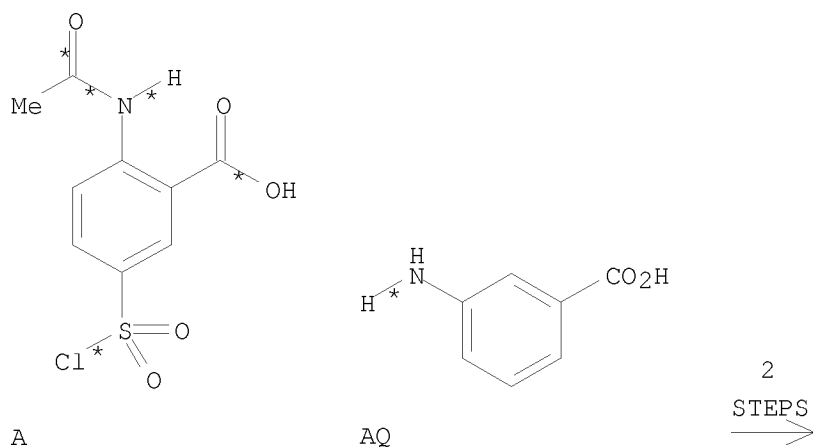
RGT D 7732-18-5 Water  
CON cooled

PRO CW 774217-40-2

NTE chemoselective

RX(170) OF 372 COMPOSED OF RX(20), RX(58)

RX(170) A + AQ ==> CX



CX  
YIELD 82%

RX(20) RCT A 181478-44-4, AQ 99-05-8

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STAGE(1)

CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO AR 774217-04-8

RX(58) RCT AR 774217-04-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

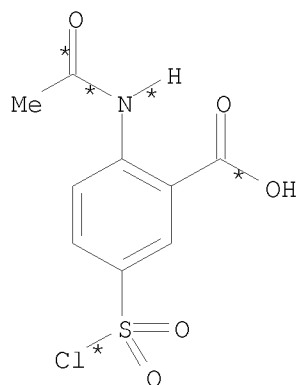
RGT D 7732-18-5 Water  
CON cooled

PRO CX 774217-41-3

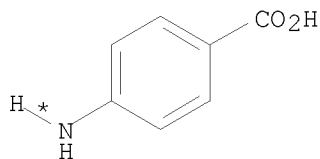
NTE chemoselective

RX(171) OF 372 COMPOSED OF RX(21), RX(59)

RX(171) A + AS ==> CY



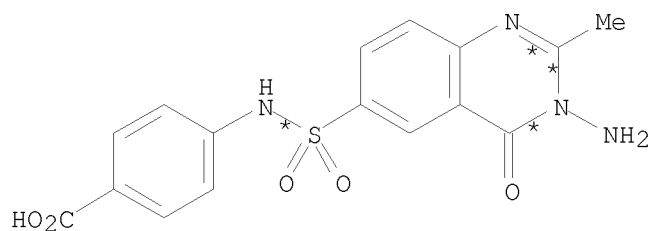
A



AS

2  
STEPS  
→

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CY  
YIELD 81%

RX(21) RCT A 181478-44-4, AS 150-13-0

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AT 774217-05-9

RX(59) RCT AT 774217-05-9

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

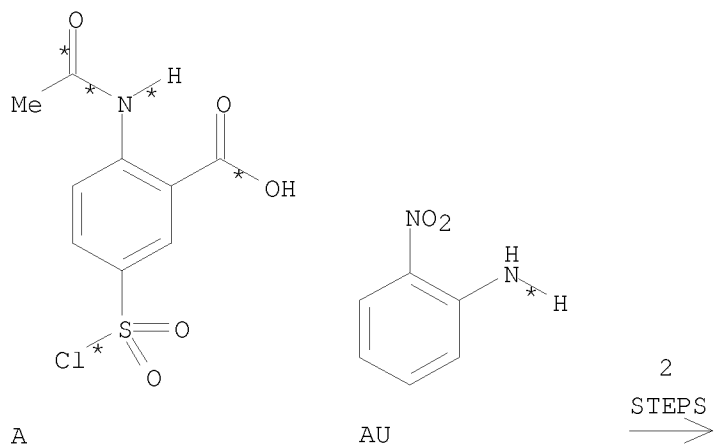
CON cooled

PRO CY 774217-42-4

NTE chemoselective

RX(172) OF 372 COMPOSED OF RX(22), RX(60)

RX(172) A + AU ==> CZ



CZ  
YIELD 78%

RX(22) RCT A 181478-44-4, AU 88-74-4

STAGE(1)

CAT 110-86-1 Pyridine  
 SOL 64-17-5 EtOH  
 CON SUBSTAGE(1) 4 hours, 120 deg C  
 SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
 CON cooled

PRO AV 774217-06-0

RX(60) RCT AV 774217-06-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
 SOL 67-56-1 MeOH  
 CON 3 hours, reflux

STAGE(2)

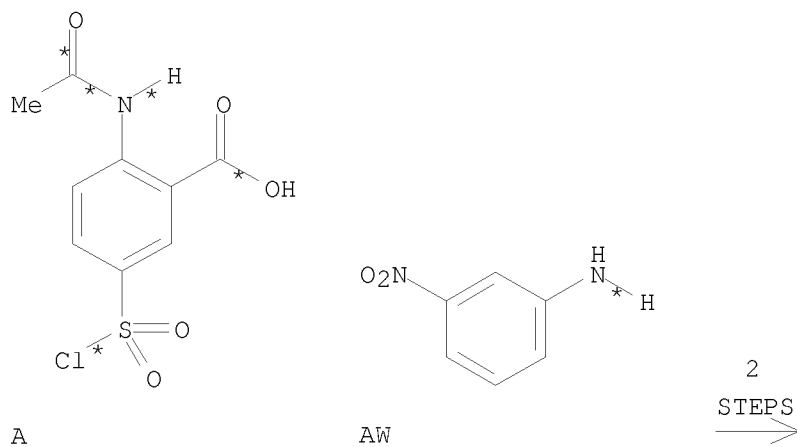
RGT D 7732-18-5 Water  
 CON cooled



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PRO CZ 774217-43-5  
NTE chemoselective

RX(173) OF 372 COMPOSED OF RX(23), RX(61)  
RX(173) A + AW ==> DA



DA  
YIELD 76%

RX(23) RCT A 181478-44-4, AW 99-09-2

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AX 774217-07-1

RX(61) RCT AX 774217-07-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

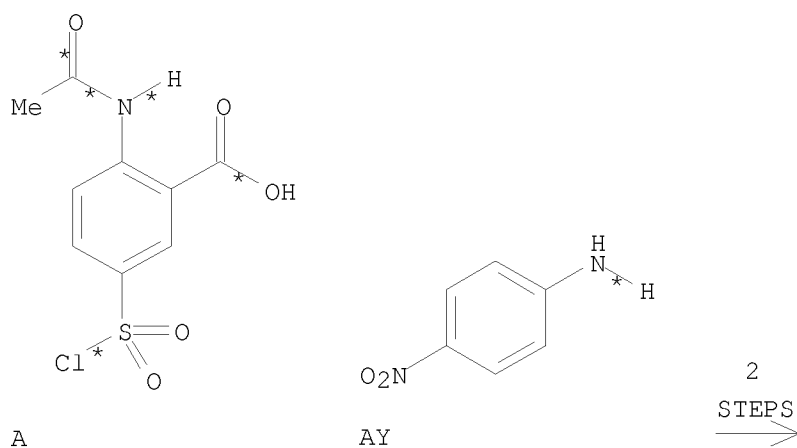
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SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DA 774217-44-6  
NTE chemoselective

RX(174) OF 372 COMPOSED OF RX(24), RX(62)  
RX(174) A + AY ==> DB



DB  
YIELD 79%

RX(24) RCT A 181478-44-4, AY 100-01-6

STAGE(1)  
CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

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PRO AZ 774217-08-2

RX(62) RCT AZ 774217-08-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

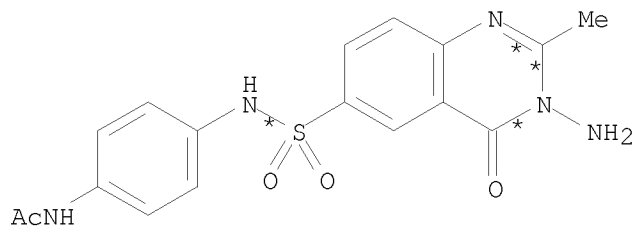
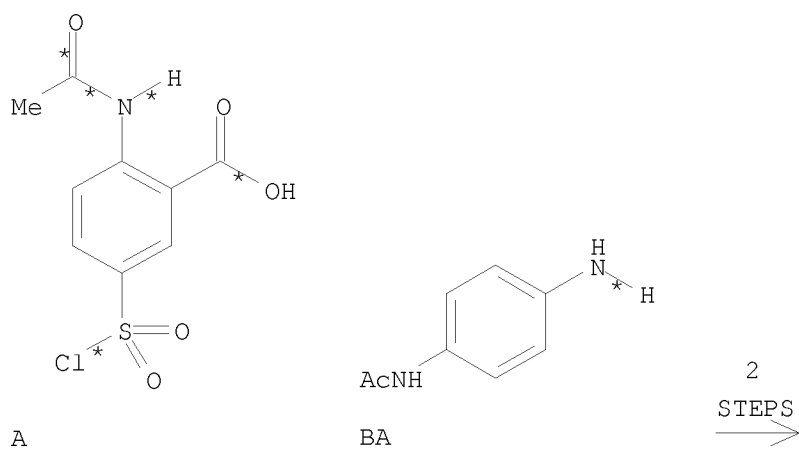
CON cooled

PRO DB 774217-45-7

NTE chemoselective

RX(175) OF 372 COMPOSED OF RX(25), RX(63)

RX(175) A + BA ==> DC



YIELD 71%

RX(25) RCT A 181478-44-4, BA 122-80-5

STAGE(1)

CAT 110-86-1 Pyridine

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SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO BB 774217-09-3

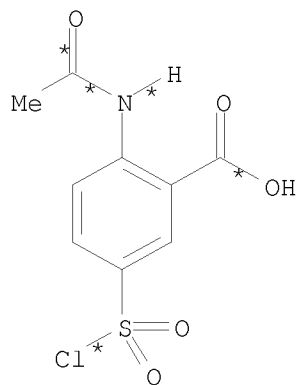
RX(63) RCT BB 774217-09-3

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

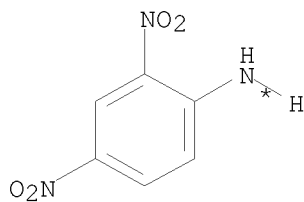
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DC 774217-46-8  
NTE chemoselective

RX(176) OF 372 COMPOSED OF RX(26), RX(64)  
RX(176) A + BC ==> DD



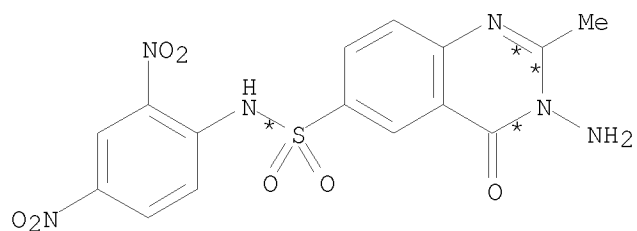
A



BC

2  
STEPS  
→

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DD  
YIELD 76%

RX(26) RCT A 181478-44-4, BC 97-02-9

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BD 774217-10-6

RX(64) RCT BD 774217-10-6

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

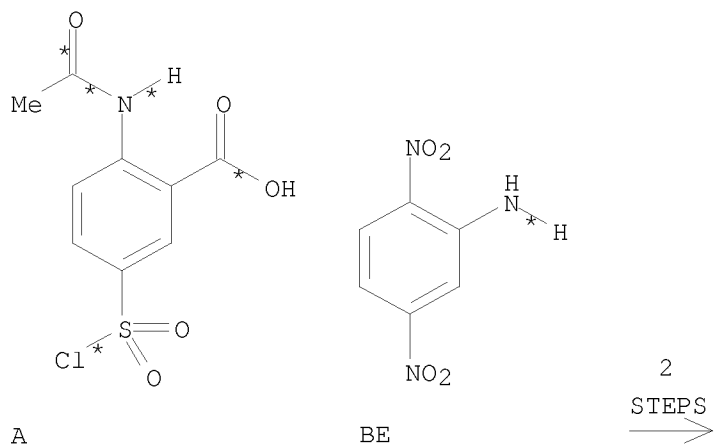
PRO DD 774217-47-9

NTE chemoselective

RX(177) OF 372 COMPOSED OF RX(27), RX(65)

RX(177) A + BE ==> DE

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DE  
YIELD 78%

RX(27) RCT A 181478-44-4, BE 619-18-1

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BF 774217-11-7

RX(65) RCT BF 774217-11-7

STAGE(1)

RGT CD 7803-57-8  $\text{N}_2\text{H}_4\cdot\text{H}_2\text{O}$

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

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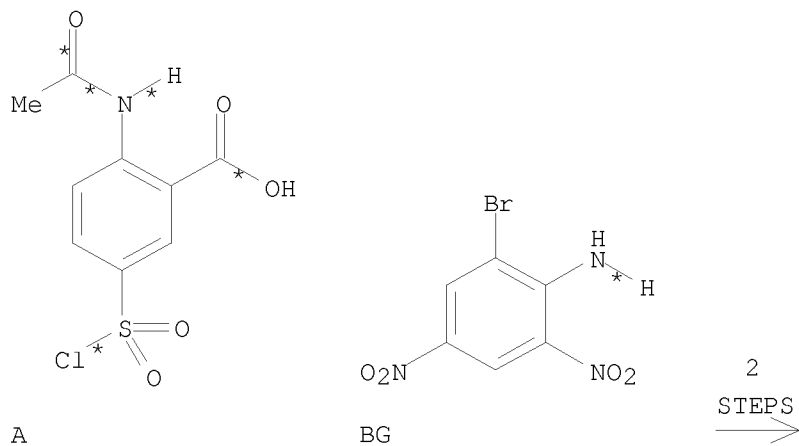
CON cooled

PRO DE 774217-48-0

NTE chemoselective

RX(178) OF 372 COMPOSED OF RX(28), RX(66)

RX(178) A + BG ==> DF



DF  
YIELD 72%

RX(28) RCT A 181478-44-4, BG 1817-73-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BH 774217-12-8

RX(66) RCT BH 774217-12-8

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STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

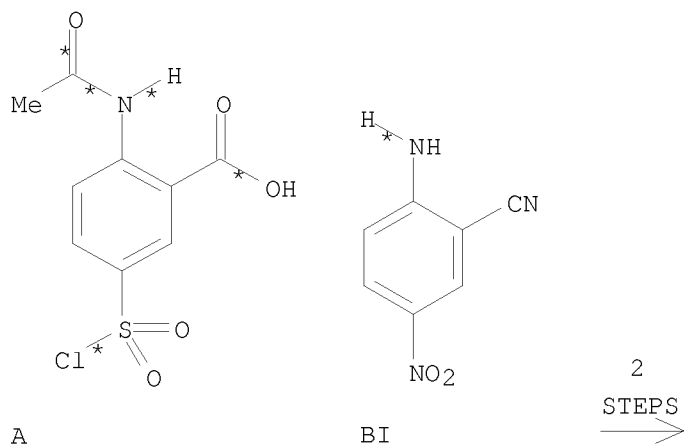
CON cooled

PRO DF 774217-49-1

NTE chemoselective

RX(179) OF 372 COMPOSED OF RX(29), RX(67)

RX(179) A + BI ==> DG



DG  
YIELD 71%

RX(29) RCT A 181478-44-4, BI 17420-30-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)



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RGT D 7732-18-5 Water  
CON cooled

PRO BJ 774217-13-9

RX(67) RCT BJ 774217-13-9

STAGE(1)

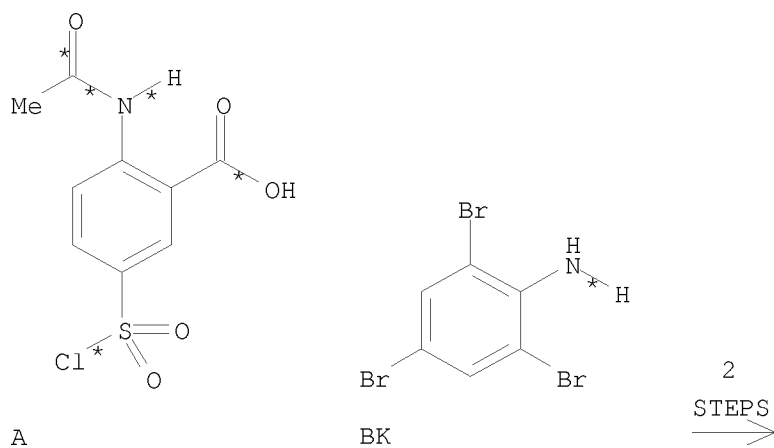
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DG 774217-50-4  
NTE chemoselective

RX(180) OF 372 COMPOSED OF RX(30), RX(68)  
RX(180) A + BK ==> DH



DH  
YIELD 80%

RX(30) RCT A 181478-44-4, BK 147-82-0

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STAGE(1)

CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO BL 774217-14-0

RX(68) RCT BL 774217-14-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

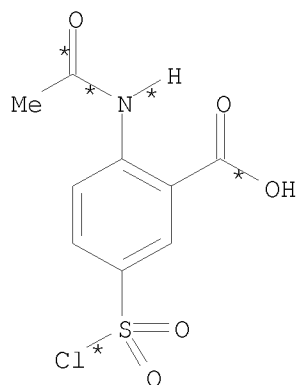
RGT D 7732-18-5 Water  
CON cooled

PRO DH 774217-51-5

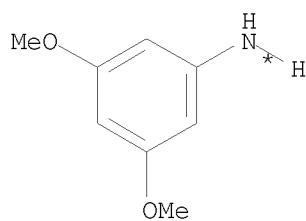
NTE chemoselective

RX(181) OF 372 COMPOSED OF RX(31), RX(69)

RX(181) A + BM ==> DI



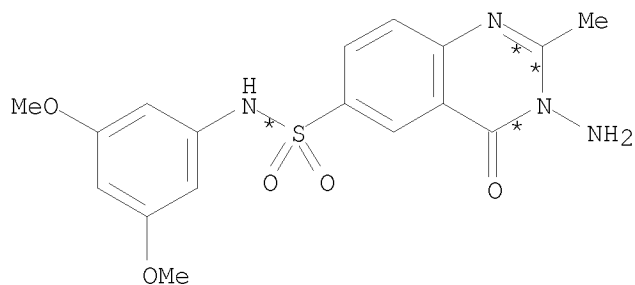
A



BM

2  
STEPS  
→

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DI  
YIELD 75%

RX(31) RCT A 181478-44-4, BM 10272-07-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BN 774217-15-1

RX(69) RCT BN 774217-15-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

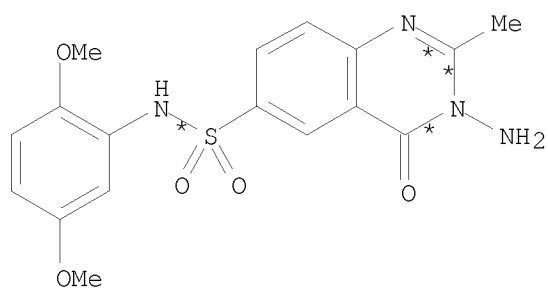
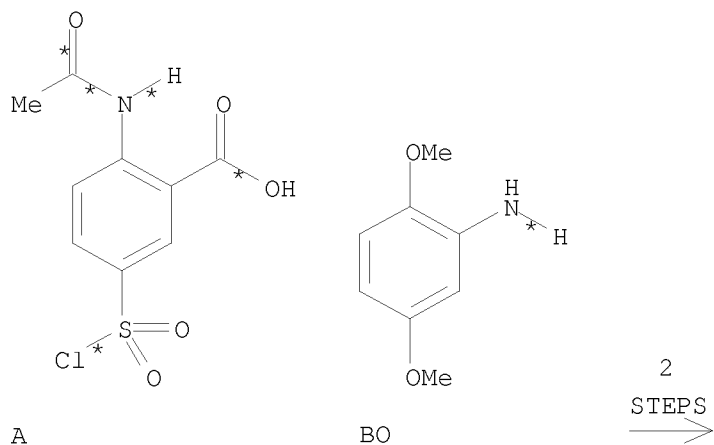
PRO DI 774217-52-6

NTE chemoselective

RX(182) OF 372 COMPOSED OF RX(32), RX(70)

RX(182) A + BO ==> DJ

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DJ  
YIELD 72%

RX(32) RCT A 181478-44-4, BO 102-56-7

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BP 774217-16-2

RX(70) RCT BP 774217-16-2

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

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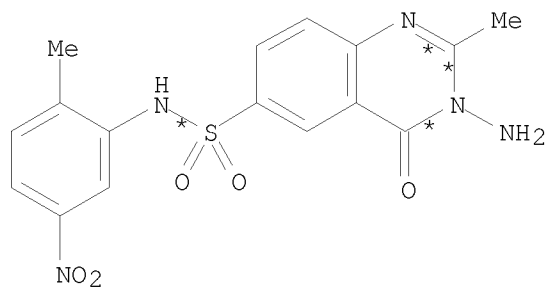
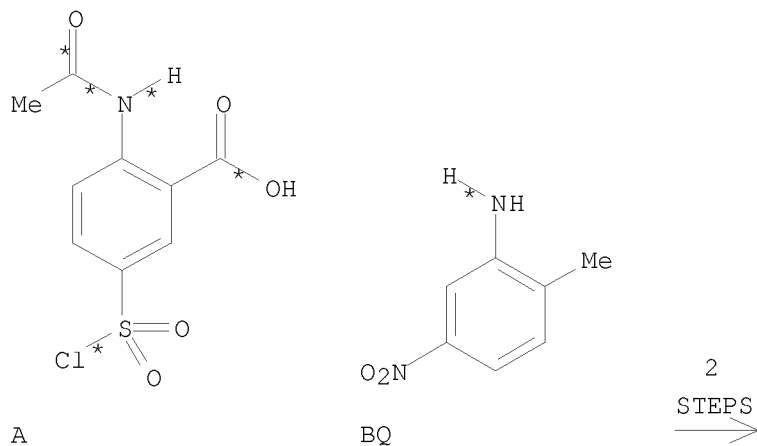
CON cooled

PRO DJ 774217-53-7

NTE chemoselective

RX(183) OF 372 COMPOSED OF RX(33), RX(71)

RX(183) A + BQ ==> DK



DK  
YIELD 68%

RX(33) RCT A 181478-44-4, BQ 99-55-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BR 774217-17-3

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RX(71) RCT BR 774217-17-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

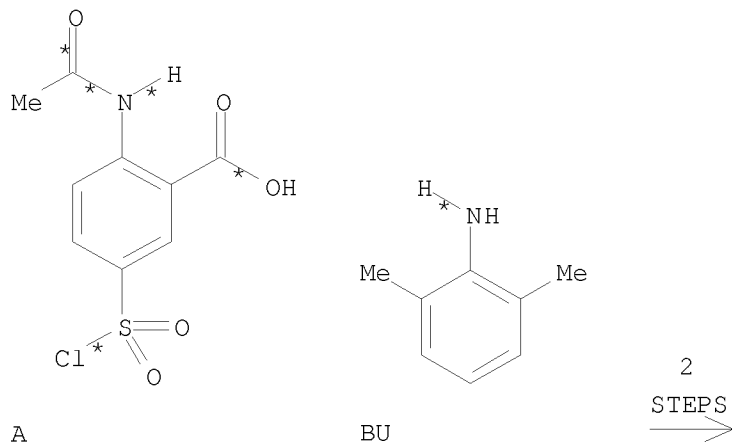
CON cooled

PRO DK 774217-54-8

NTE chemoselective

RX(184) OF 372 COMPOSED OF RX(35), RX(72)

RX(184) A + BU ==> DL



DL  
YIELD 72%

RX(35) RCT A 181478-44-4, BU 87-62-7

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

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STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO BV 774217-19-5

RX(72) RCT BV 774217-19-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

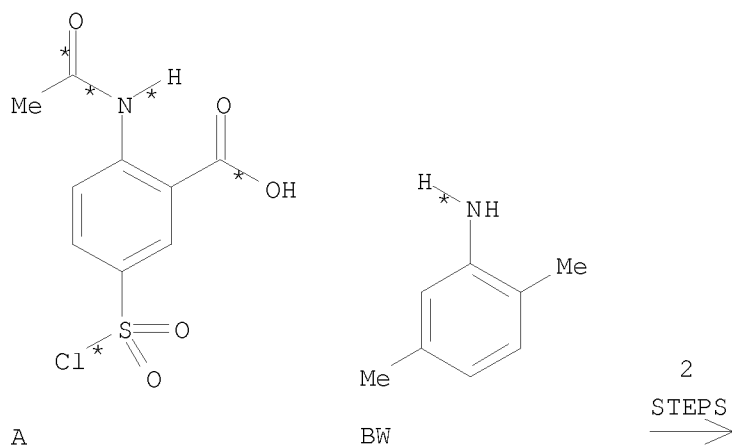
RGT D 7732-18-5 Water  
CON cooled

PRO DL 774217-56-0

NTE chemoselective

RX(185) OF 372 COMPOSED OF RX(36), RX(73)

RX(185) A + BW ==> DM



DM  
YIELD 70%

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RX(36) RCT A 181478-44-4, BW 95-78-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BX 774217-20-8

RX(73) RCT BX 774217-20-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

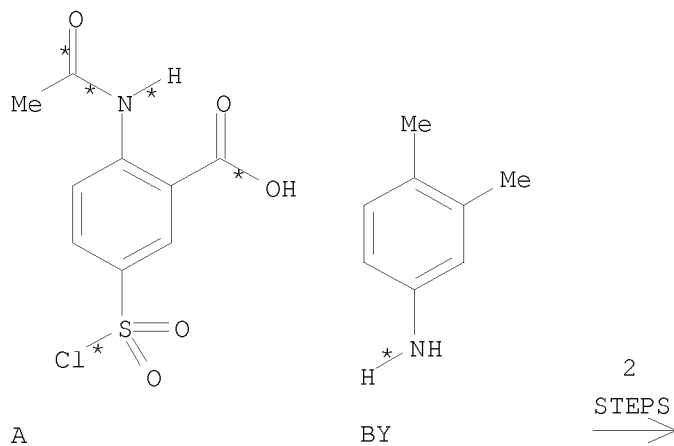
CON cooled

PRO DM 774217-57-1

NTE chemoselective

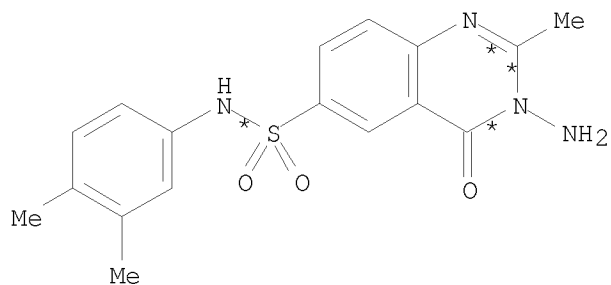
RX(186) OF 372 COMPOSED OF RX(37), RX(74)

RX(186) A + BY ==> DN





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DN  
YIELD 75%

RX(37) RCT A 181478-44-4, BY 95-64-7

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BZ 774217-21-9

RX(74) RCT BZ 774217-21-9

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

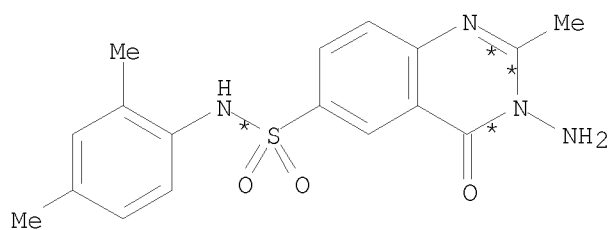
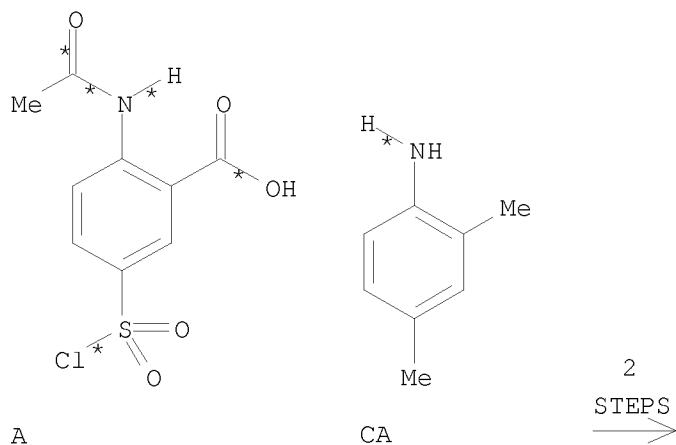
PRO DN 774217-58-2

NTE chemoselective

RX(187) OF 372 COMPOSED OF RX(38), RX(75)

RX(187) A + CA ==> DO

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DO  
YIELD 77%

RX(38) RCT A 181478-44-4, CA 95-68-1

STAGE(1)

CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CB 774217-22-0

RX(75) RCT CB 774217-22-0

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

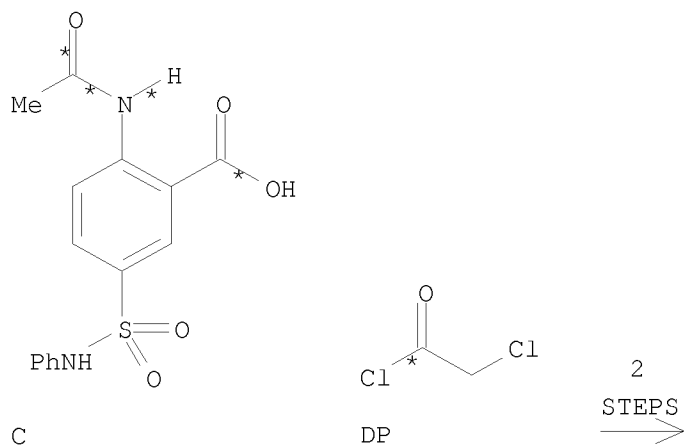
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

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PRO DO 774217-59-3  
NTE chemoselective

RX(188) OF 372 COMPOSED OF RX(39), RX(76)  
RX(188) C + DP ==> DQ



DQ  
YIELD 61%

RX(39) RCT C 774216-86-3

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CC 774217-23-1  
NTE chemoselective

RX(76) RCT CC 774217-23-1, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH

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CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

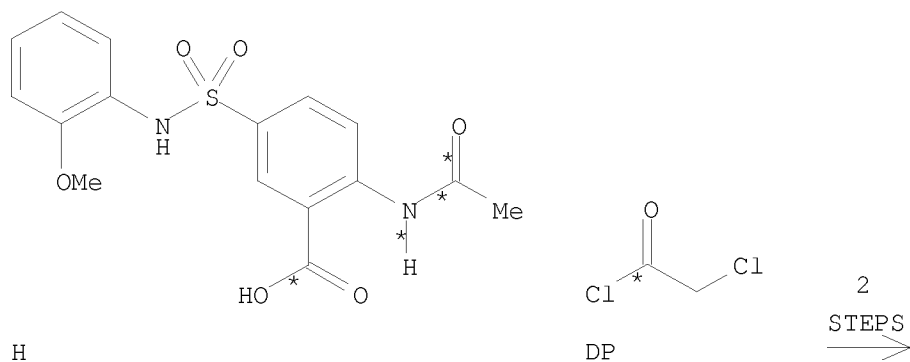
RGT D 7732-18-5 Water

CON cooled

PRO DQ 774217-60-6

RX(189) OF 372 COMPOSED OF RX(40), RX(77)

RX(189) H + DP ==> DR



DR  
YIELD 59%

RX(40) RCT H 774216-87-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CF 774217-24-2

NTE chemoselective

RX(77) RCT CF 774217-24-2, DP 79-04-9

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STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

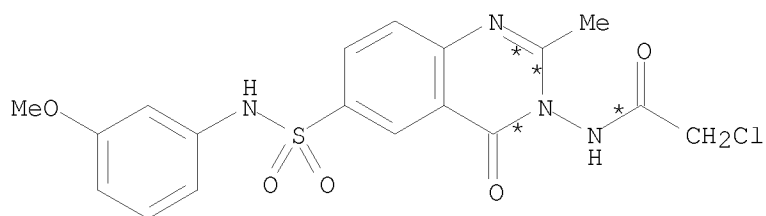
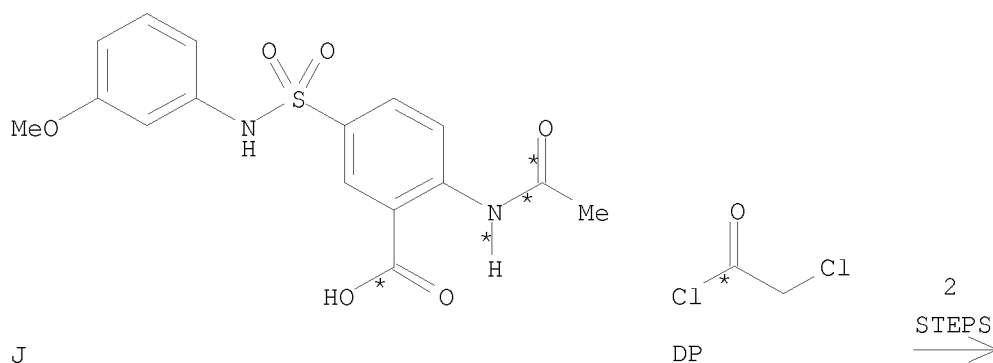
RGT D 7732-18-5 Water

CON cooled

PRO DR 774217-61-7

RX(190) OF 372 COMPOSED OF RX(41), RX(78)

RX(190) J + DP ==> DS



DS  
YIELD 53%

RX(41) RCT J 774216-88-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CG 774217-25-3

NTE chemoselective

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RX(78) RCT CG 774217-25-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

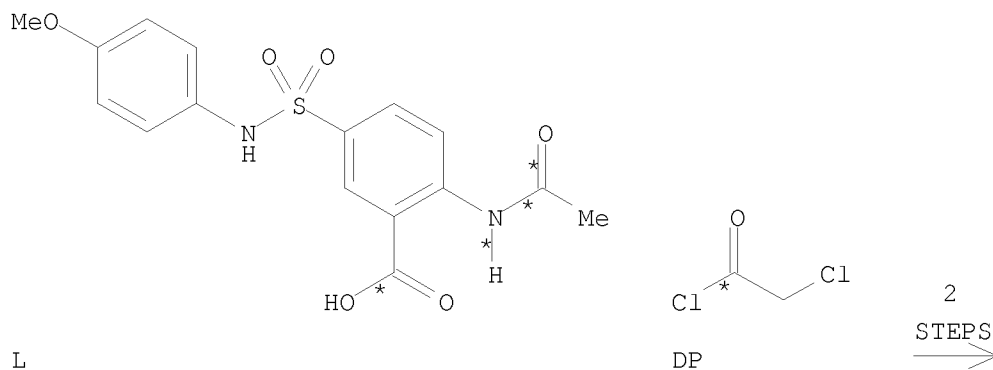
RGT D 7732-18-5 Water

CON cooled

PRO DS 774217-62-8

RX(191) OF 372 COMPOSED OF RX(42), RX(79)

RX(191) L + DP ==> DT



DT  
YIELD 63%

RX(42) RCT L 774216-89-6

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

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PRO CH 774217-26-4  
NTE chemoselective

RX(79) RCT CH 774217-26-4, DP 79-04-9

STAGE(1)

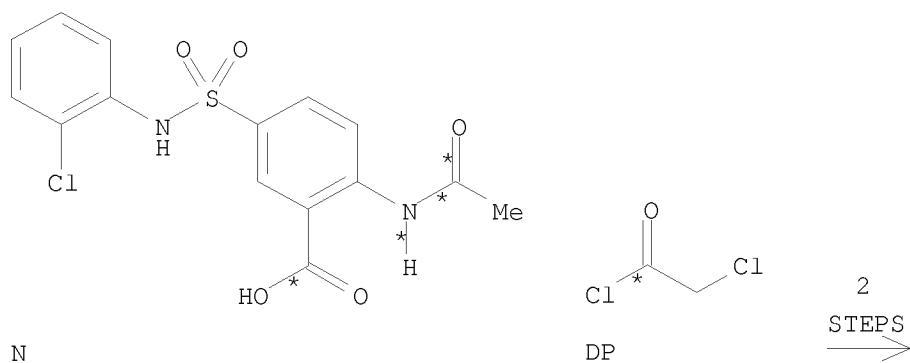
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DT 774217-63-9

RX(192) OF 372 COMPOSED OF RX(43), RX(80)  
RX(192) N + DP ==> DU



DU  
YIELD 53%

RX(43) RCT N 774216-90-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

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STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CI 774217-27-5  
NTE chemoselective

RX(80) RCT CI 774217-27-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

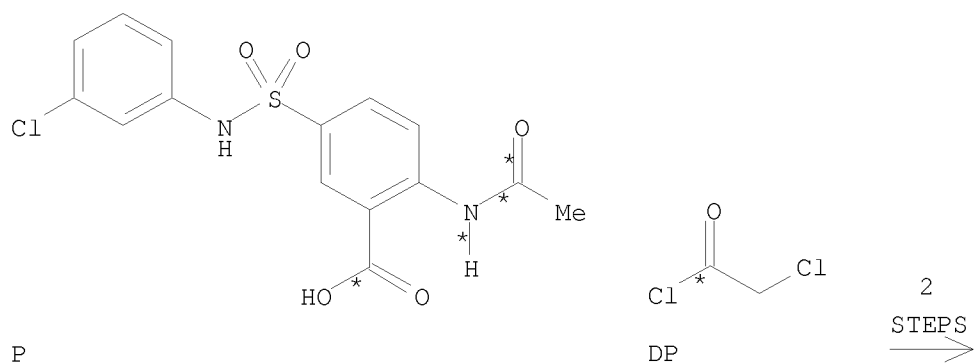
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DU 774217-64-0

RX(193) OF 372 COMPOSED OF RX(44), RX(81)

RX(193) P + DP ==> DV



DV  
YIELD 59%

RX(44) RCT P 774216-91-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O



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SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CJ 774217-28-6  
NTE chemoselective

RX(81) RCT CJ 774217-28-6, DP 79-04-9

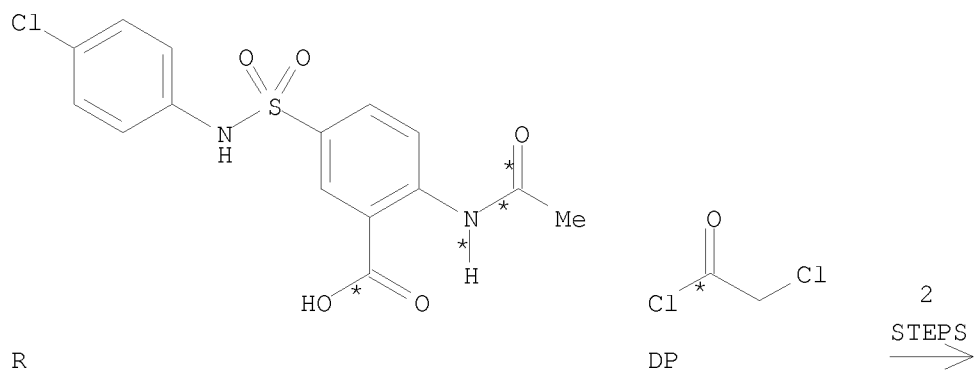
STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DV 774217-65-1

RX(194) OF 372 COMPOSED OF RX(45), RX(82)

RX(194) R + DP ==> DW



DW  
YIELD 58%

RX(45) RCT R 774216-92-1

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STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CK 774217-29-7  
NTE chemoselective

RX(82) RCT CK 774217-29-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

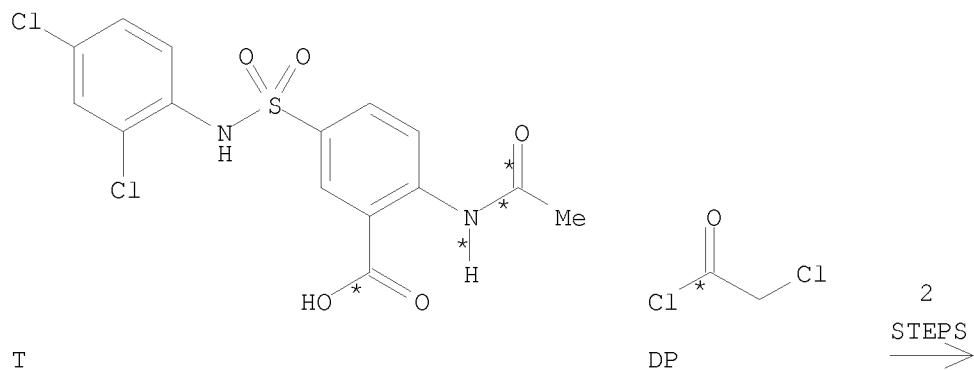
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DW 774217-66-2

RX(195) OF 372 COMPOSED OF RX(46), RX(83)

RX(195) T + DP ==> DX



DX  
YIELD 63%

RX (46) RCT T 774216-93-2

STAGE (1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE (2)

RGT D 7732-18-5 Water

CON    cooled

PRO CL 774217-30-0

NTE chemoselective

RX(83) RCT CL 774217-30-0, DP 79-04-9

STAGE (1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE (2) cooled

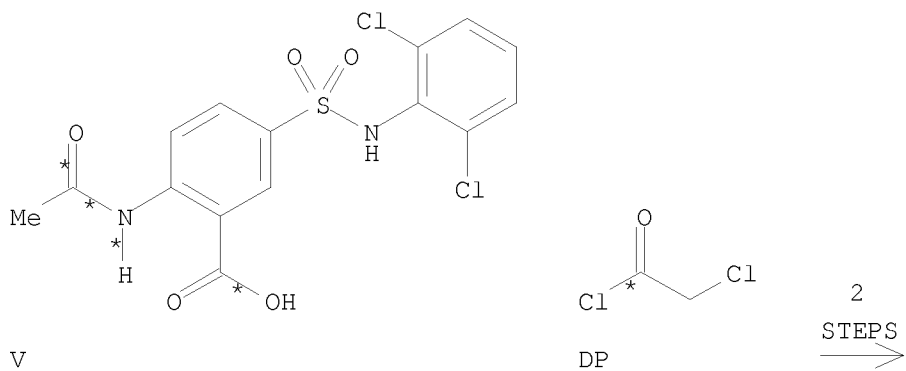
STAGE (2)

RGT D 7732-18-5 Water

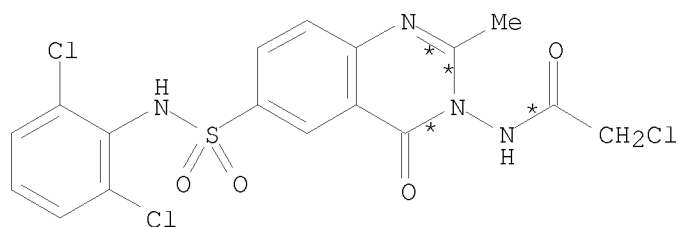
CON    cooled

PRO DX 774217-67-3

RX(196) OF 372 COMPOSED OF RX(47), RX(84)

$$\text{RX(196)} \quad \text{V} \quad + \quad \text{DP} \quad \Longrightarrow \quad \text{DY}$$


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DY  
YIELD 57%

RX(47) RCT V 774216-94-3

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CM 774217-31-1  
NTE chemoselective

RX(84) RCT CM 774217-31-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

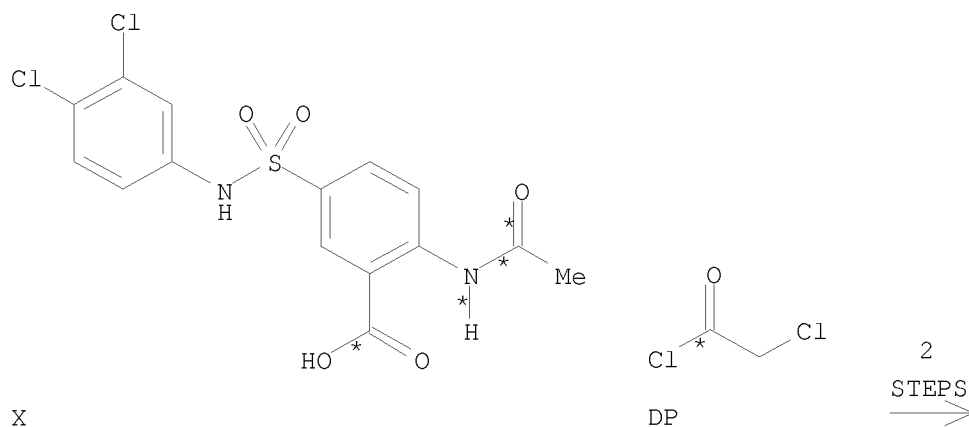
RGT D 7732-18-5 Water  
CON cooled

PRO DY 774217-68-4

RX(197) OF 372 COMPOSED OF RX(48), RX(85)

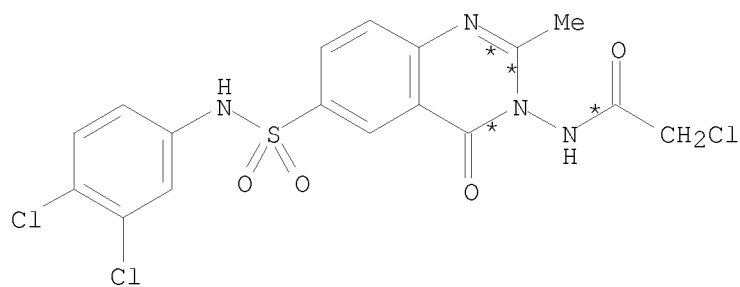
RX(197) X + DP ==> DZ

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X

DP



DZ  
YIELD 57%

RX(48) RCT X 774216-95-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CN 774217-32-2  
NTE chemoselective

RX(85) RCT CN 774217-32-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

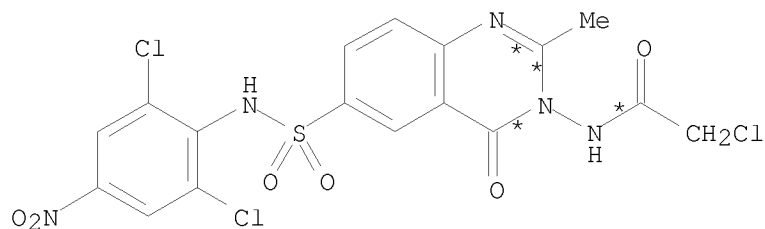
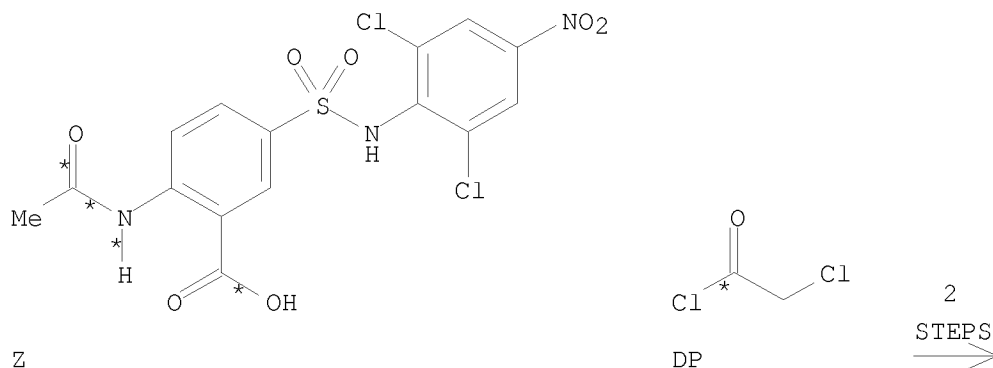
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CON cooled

PRO DZ 774217-69-5

RX(198) OF 372 COMPOSED OF RX(49), RX(86)

RX(198) Z + DP ==> EA



EA  
YIELD 62%

RX(49) RCT Z 218617-81-3

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CO 234096-58-3

NTE chemoselective

RX(86) RCT CO 234096-58-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

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STAGE(2)

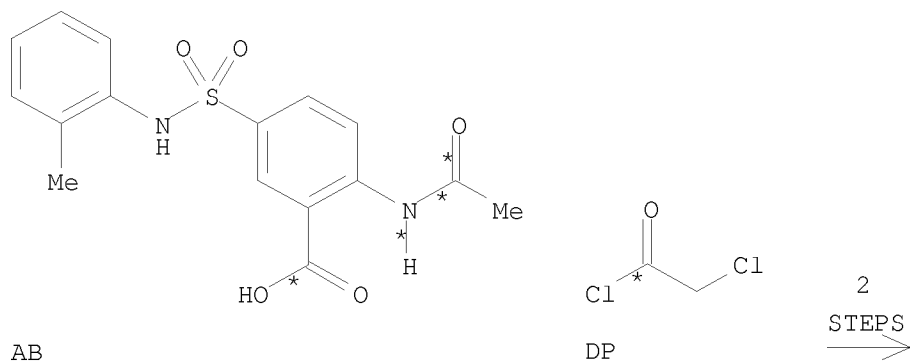
RGT D 7732-18-5 Water

CON cooled

PRO EA 774217-70-8

RX(199) OF 372 COMPOSED OF RX(50), RX(87)

RX(199) AB + DP ==> EB



EB  
YIELD 59%

RX(50) RCT AB 774216-96-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CP 774217-33-3

NTE chemoselective

RX(87) RCT CP 774217-33-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

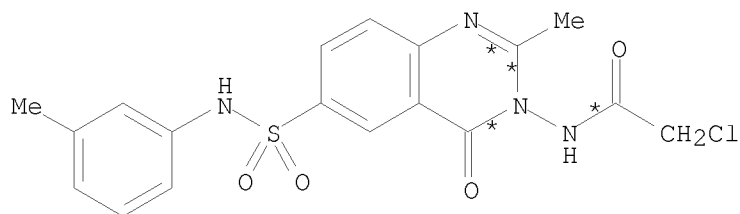
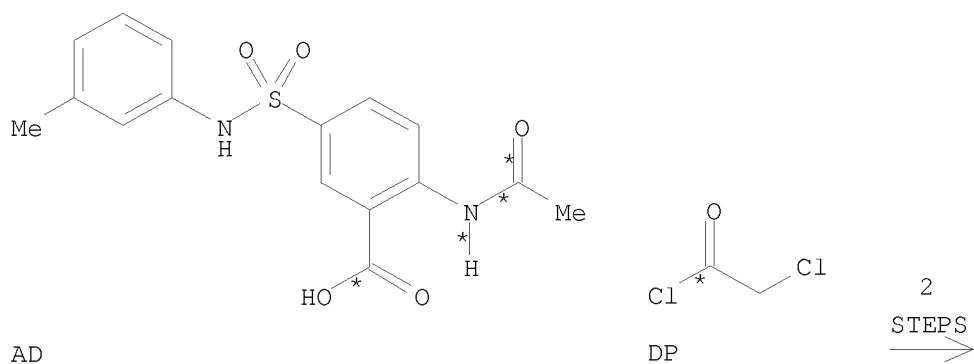
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SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EB 774217-71-9

RX(200) OF 372 COMPOSED OF RX(51), RX(88)  
RX(200) AD + DP ==> EC



EC  
YIELD 64%

RX(51) RCT AD 774216-97-6

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CQ 774217-34-4  
NTE chemoselective

RX(88) RCT CQ 774217-34-4, DP 79-04-9



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STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

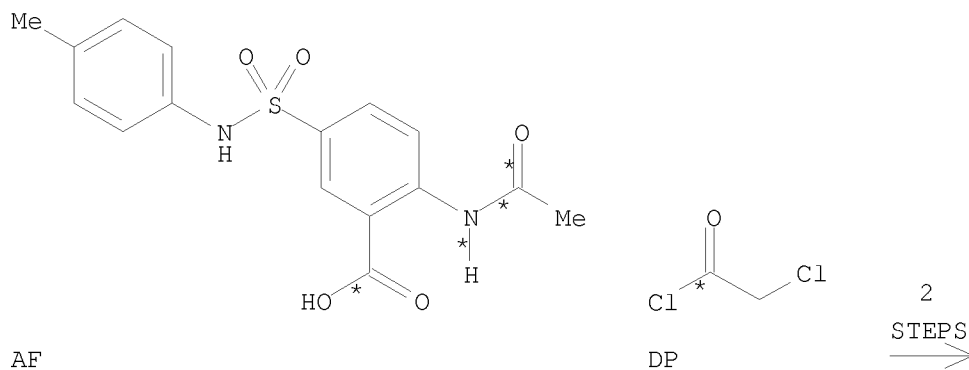
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EC 774217-72-0

RX(201) OF 372 COMPOSED OF RX(52), RX(89)

RX(201) AF + DP ==> ED



ED  
YIELD 63%

RX(52) RCT AF 774216-98-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CR 774217-35-5

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NTE chemoselective

RX(89) RCT CR 774217-35-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

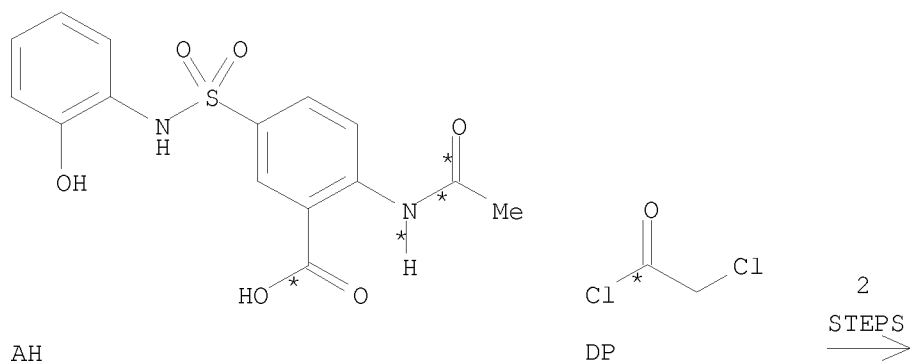
RGT D 7732-18-5 Water

CON cooled

PRO ED 774217-73-1

RX(202) OF 372 COMPOSED OF RX(53), RX(90)

RX(202) AH + DP ==> EE



EE  
YIELD 58%

RX(53) RCT AH 774216-99-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

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CON cooled

PRO CS 774217-36-6

NTE chemoselective

RX(90) RCT CS 774217-36-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

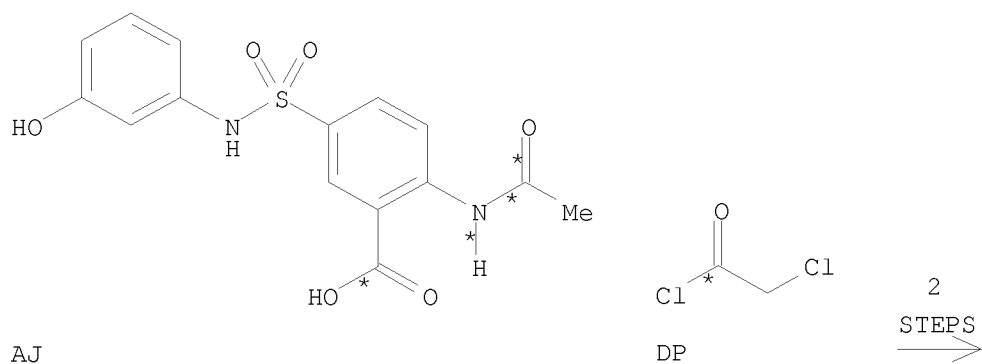
RGT D 7732-18-5 Water

CON cooled

PRO EE 774217-74-2

RX(203) OF 372 COMPOSED OF RX(54), RX(91)

RX(203) AJ + DP ==> EF



EF  
YIELD 59%

RX(54) RCT AJ 774217-00-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

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STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CT 774217-37-7

NTE chemoselective

RX(91) RCT CT 774217-37-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

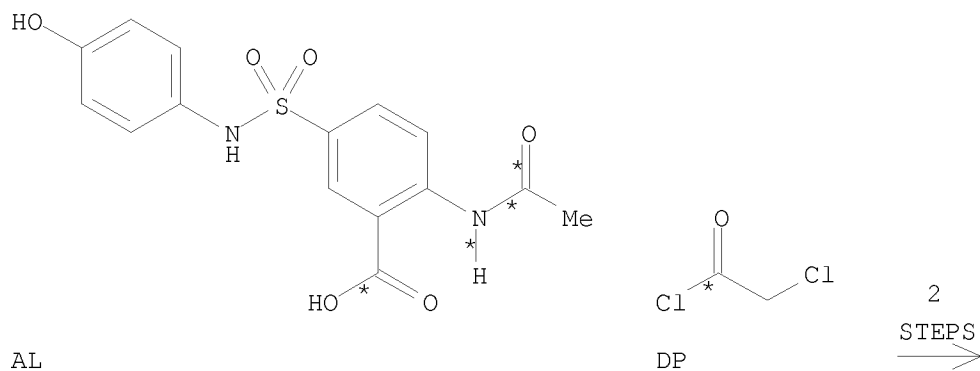
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EF 774217-75-3

RX(204) OF 372 COMPOSED OF RX(55), RX(92)

RX(204) AL + DP ==> EG



EG  
YIELD 63%

RX(55) RCT AL 774217-01-5

STAGE(1)

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RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CU 774217-38-8  
NTE chemoselective

RX(92) RCT CU 774217-38-8, DP 79-04-9

STAGE(1)

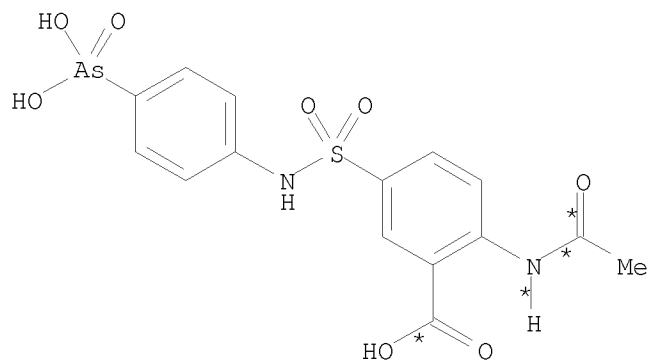
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

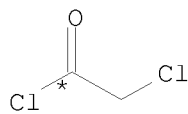
RGT D 7732-18-5 Water  
CON cooled

PRO EG 774217-76-4

RX(205) OF 372 COMPOSED OF RX(56), RX(93)  
RX(205) AN + DP ==> EH



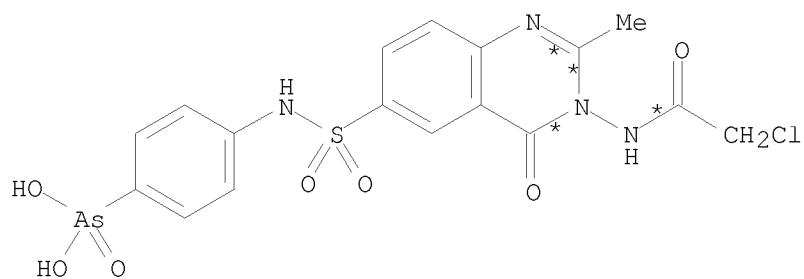
AN



DP

2  
STEPS  
→

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EH  
YIELD 71%

RX(56) RCT AN 774217-02-6

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CV 774217-39-9

NTE chemoselective

RX(93) RCT CV 774217-39-9, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

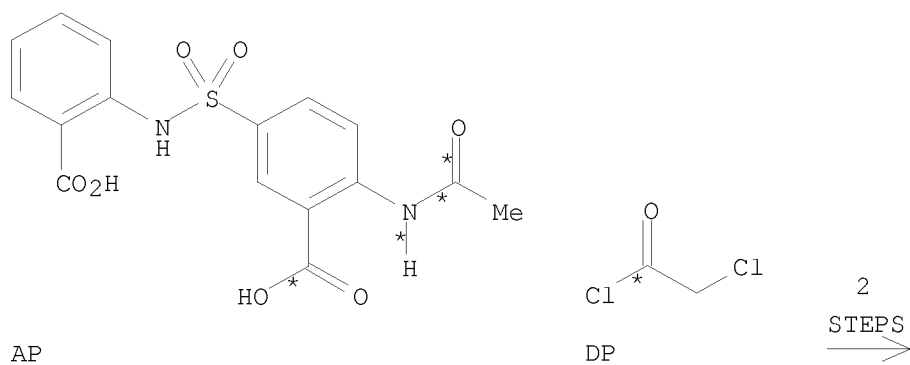
CON cooled

PRO EH 774217-77-5

RX(206) OF 372 COMPOSED OF RX(57), RX(94)

RX(206) AP + DP ==> EI

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EI  
YIELD 75%

RX(57) RCT AP 774217-03-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CW 774217-40-2

NTE chemoselective

RX(94) RCT CW 774217-40-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

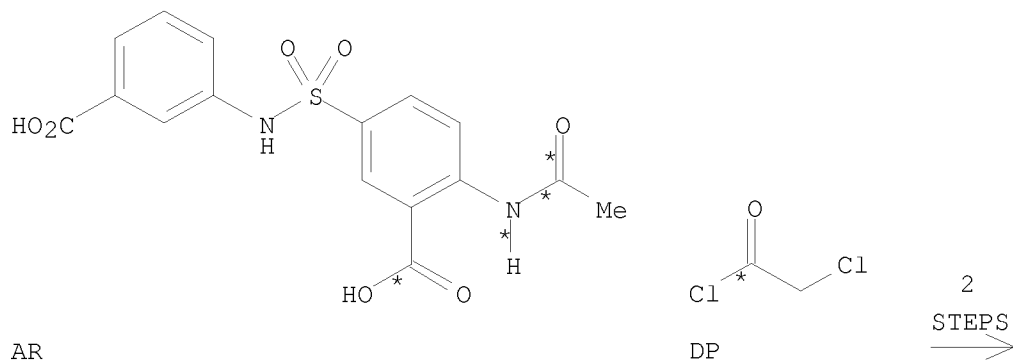
CON cooled

PRO EI 774217-78-6

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RX(207) OF 372 COMPOSED OF RX(58), RX(95)

RX(207) AR + DP ==> EJ



EJ  
YIELD 70%

RX(58) RCT AR 774217-04-8

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CX 774217-41-3  
NTE chemoselective

RX(95) RCT CX 774217-41-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

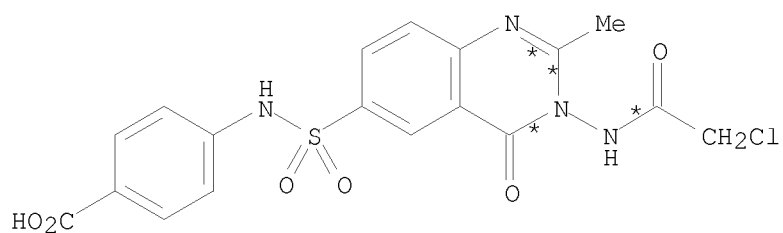
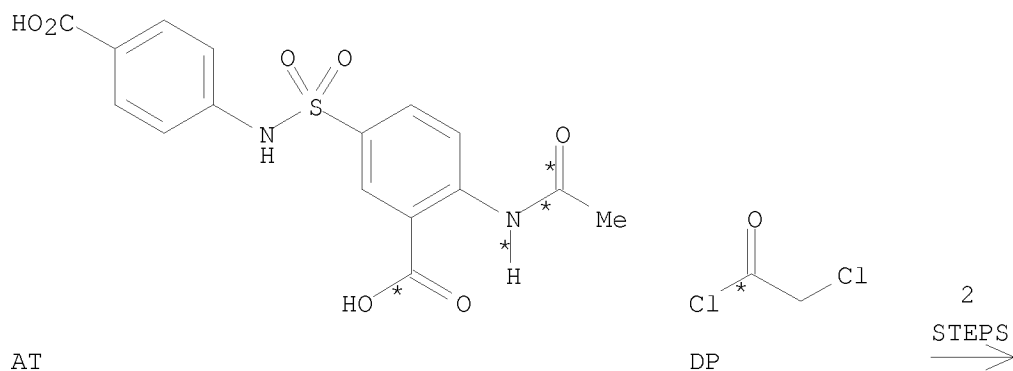


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PRO EJ 774217-79-7

RX(208) OF 372 COMPOSED OF RX(59), RX(96)

RX(208) AT + DP ==> EK



EK  
YIELD 68%

RX(59) RCT AT 774217-05-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CY 774217-42-4

NTE chemoselective

RX(96) RCT CY 774217-42-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

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STAGE(2)

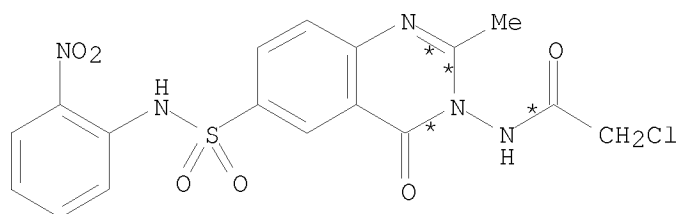
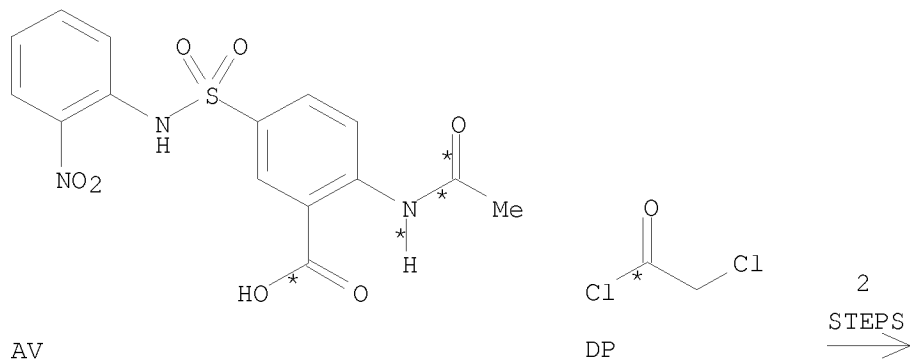
RGT D 7732-18-5 Water

CON cooled

PRO EK 774217-80-0

RX(209) OF 372 COMPOSED OF RX(60), RX(97)

RX(209) AV + DP ==> EL



EL  
YIELD 75%

RX(60) RCT AV 774217-06-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CZ 774217-43-5

NTE chemoselective

RX(97) RCT CZ 774217-43-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

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CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

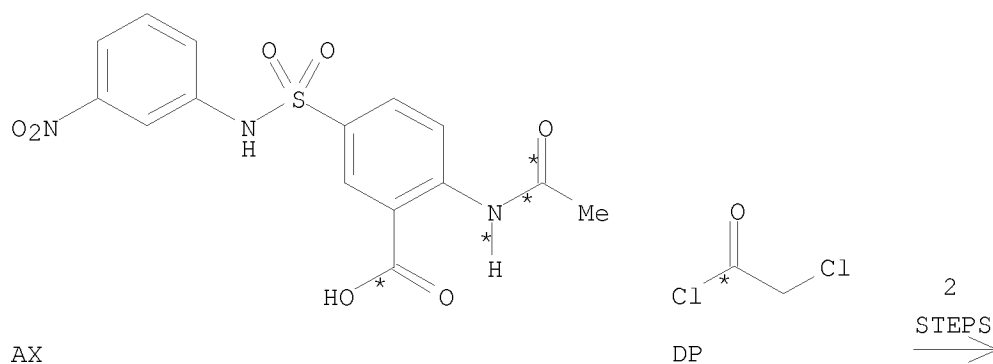
RGT D 7732-18-5 Water

CON cooled

PRO EL 774217-81-1

RX(210) OF 372 COMPOSED OF RX(61), RX(98)

RX(210) AX + DP ==> EM



EM  
YIELD 78%

RX(61) RCT AX 774217-07-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DA 774217-44-6

NTE chemoselective

RX(98) RCT DA 774217-44-6, DP 79-04-9

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STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

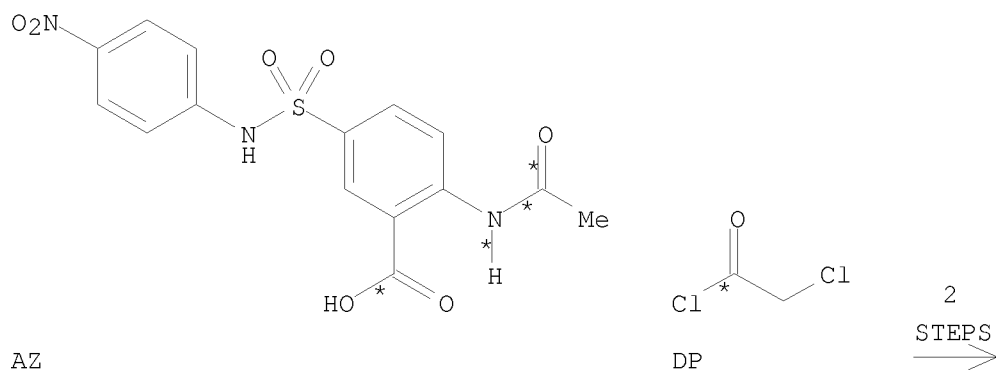
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EM 774217-82-2

RX(211) OF 372 COMPOSED OF RX(62), RX(99)

RX(211) AZ + DP ==> EN



EN  
YIELD 71%

RX(62) RCT AZ 774217-08-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DB 774217-45-7

NTE chemoselective

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RX(99) RCT DB 774217-45-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

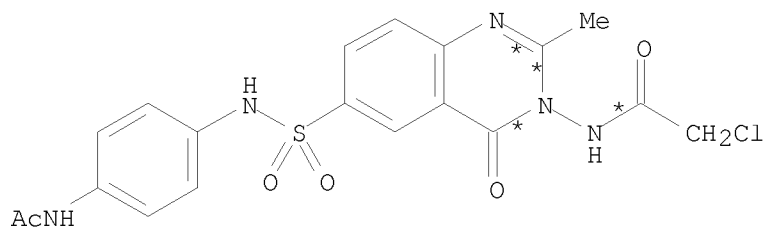
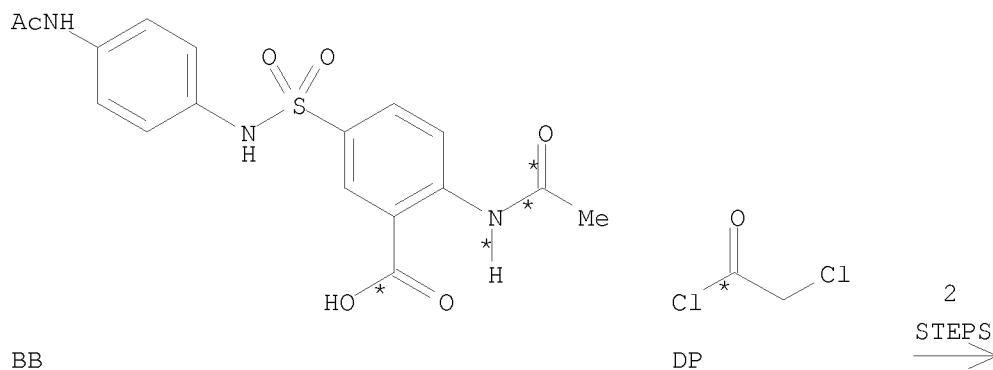
RGT D 7732-18-5 Water

CON cooled

PRO EN 774217-83-3

RX(212) OF 372 COMPOSED OF RX(63), RX(100)

RX(212) BB + DP ==> EO



EO  
YIELD 53%

RX(63) RCT BB 774217-09-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

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PRO DC 774217-46-8  
NTE chemoselective

RX(100) RCT DC 774217-46-8, DP 79-04-9

STAGE(1)

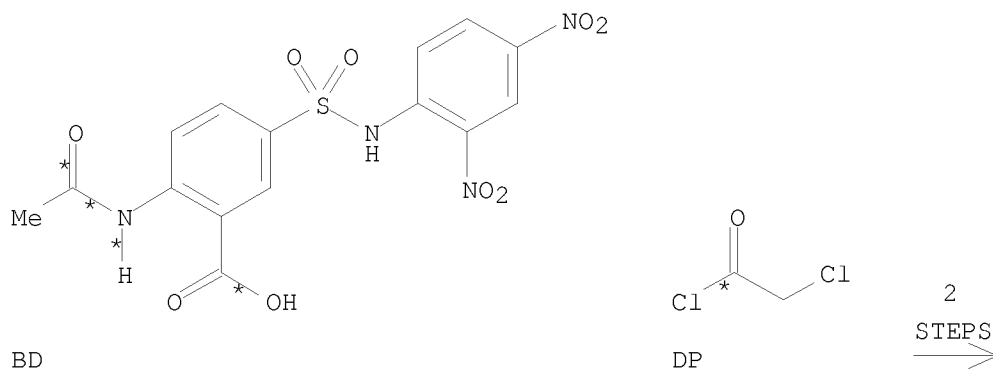
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EO 774217-84-4

RX(213) OF 372 COMPOSED OF RX(64), RX(101)  
RX(213) BD + DP ==> EP



EP  
YIELD 57%

RX(64) RCT BD 774217-10-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

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STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DD 774217-47-9  
NTE chemoselective

RX(101) RCT DD 774217-47-9, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

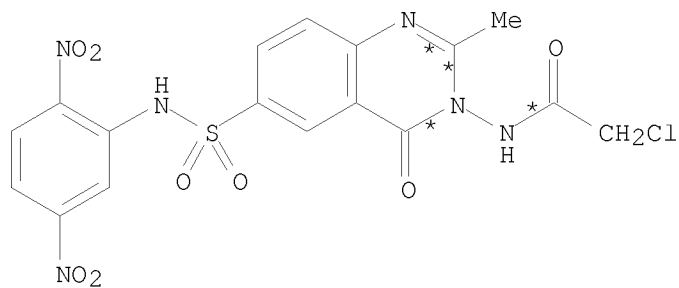
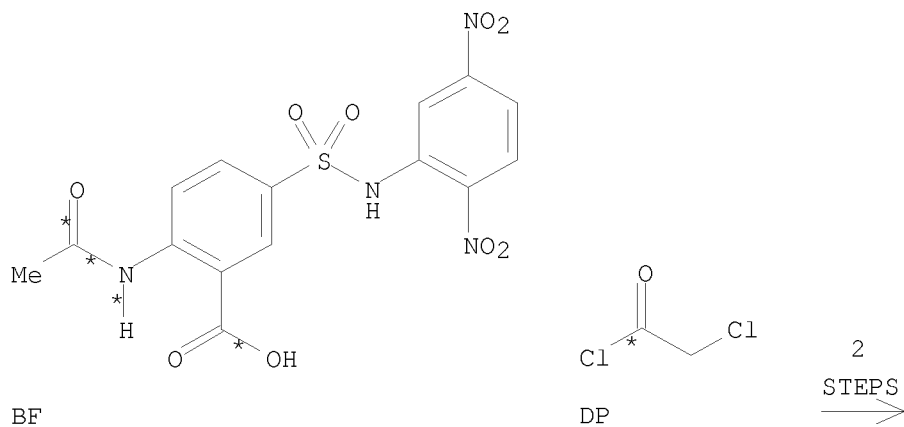
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EP 774217-85-5

RX(214) OF 372 COMPOSED OF RX(65), RX(102)

RX(214) BF + DP ==> EQ



EQ  
YIELD 57%

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RX(65) RCT BF 774217-11-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DE 774217-48-0

NTE chemoselective

RX(102) RCT DE 774217-48-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

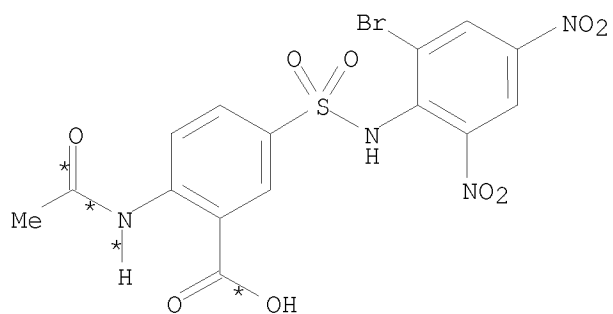
RGT D 7732-18-5 Water

CON cooled

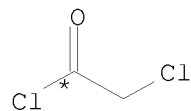
PRO EQ 774217-86-6

RX(215) OF 372 COMPOSED OF RX(66), RX(103)

RX(215) BH + DP ==> ER



BH

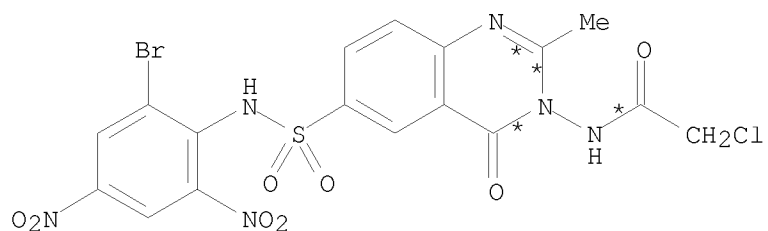


DP

2  
STEPS  
→



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ER  
YIELD 54%

RX(66) RCT BH 774217-12-8

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DF 774217-49-1  
NTE chemoselective

RX(103) RCT DF 774217-49-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

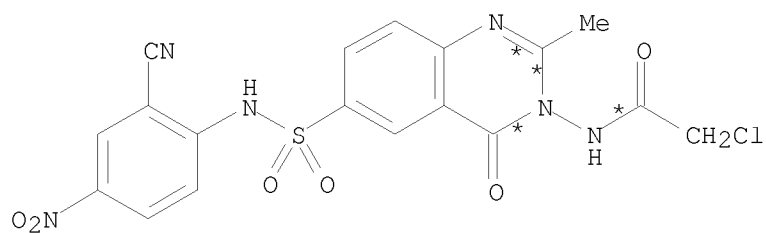
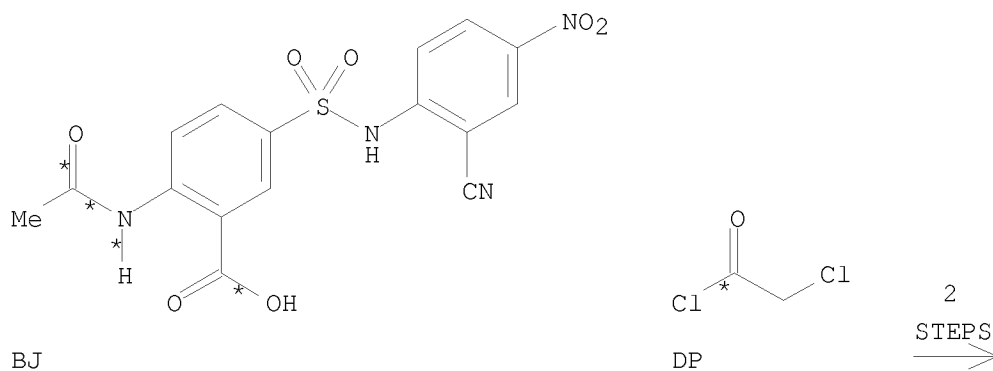
RGT D 7732-18-5 Water  
CON cooled

PRO ER 774217-87-7

RX(216) OF 372 COMPOSED OF RX(67), RX(104)

RX(216) BJ + DP ==> ES

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ES  
YIELD 51%

RX(67) RCT BJ 774217-13-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DG 774217-50-4  
NTE chemoselective

RX(104) RCT DG 774217-50-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

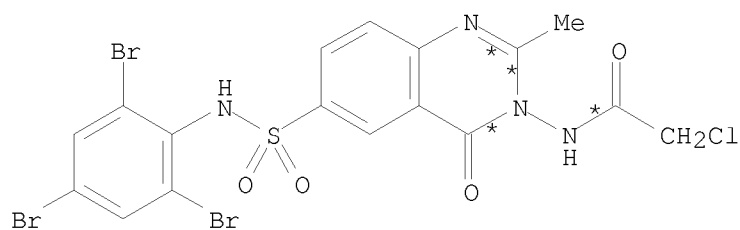
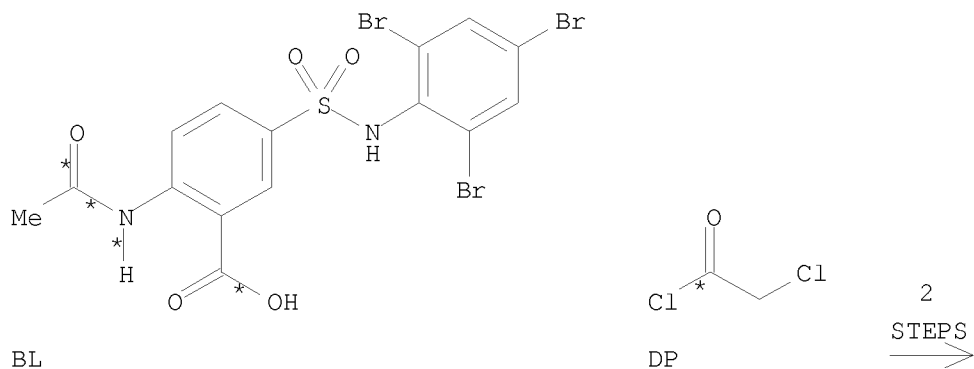
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO ES 774217-88-8

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RX(217) OF 372 COMPOSED OF RX(68), RX(105)  
RX(217) BL + DP ==> ET



ET  
YIELD 58%

RX(68) RCT BL 774217-14-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DH 774217-51-5  
NTE chemoselective

RX(105) RCT DH 774217-51-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

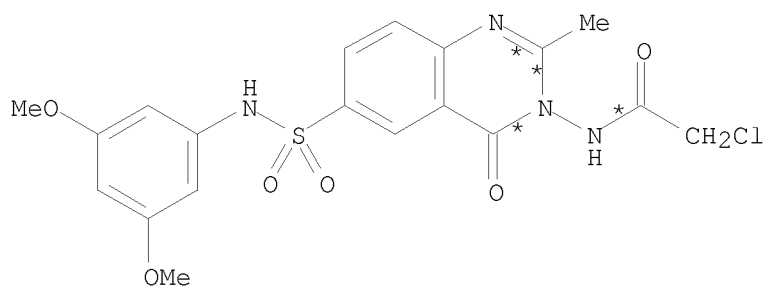
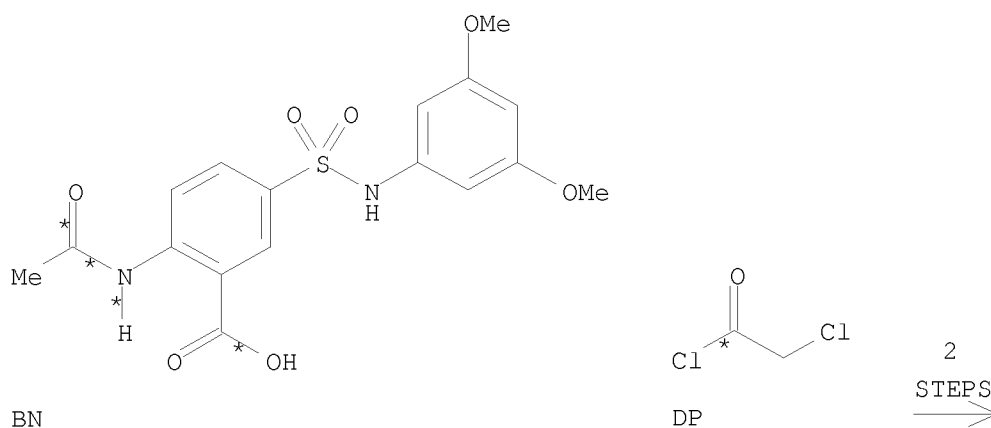
RGT D 7732-18-5 Water  
CON cooled

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PRO ET 774217-89-9

RX(218) OF 372 COMPOSED OF RX(69), RX(106)

RX(218) BN + DP ==> EU



EU  
YIELD 63%

RX(69) RCT BN 774217-15-1

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DI 774217-52-6

NTE chemoselective

RX(106) RCT DI 774217-52-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

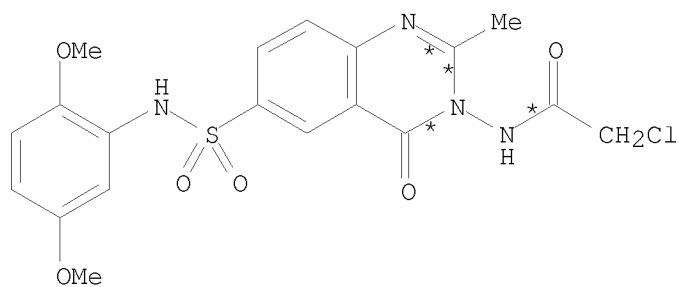
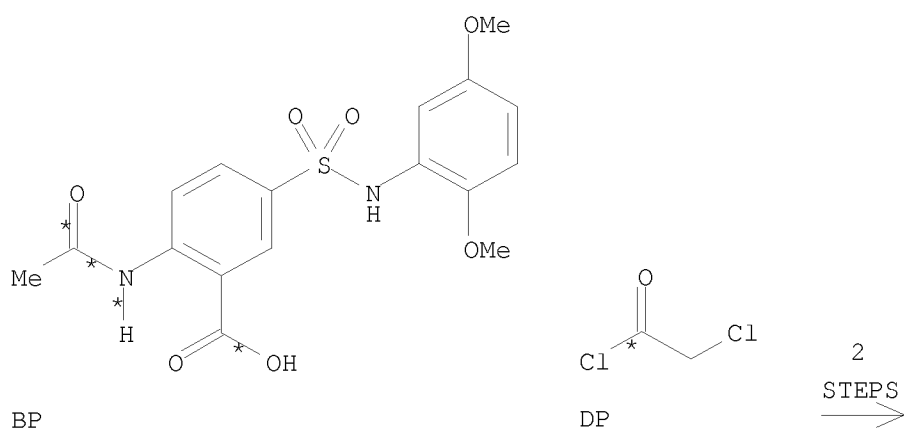
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SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EU 774217-90-2

RX(219) OF 372 COMPOSED OF RX(70), RX(107)  
RX(219) BP + DP ==> EV



YIELD 63%

RX(70) RCT BP 774217-16-2

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

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PRO DJ 774217-53-7  
NTE chemoselective

RX(107) RCT DJ 774217-53-7, DP 79-04-9

STAGE(1)

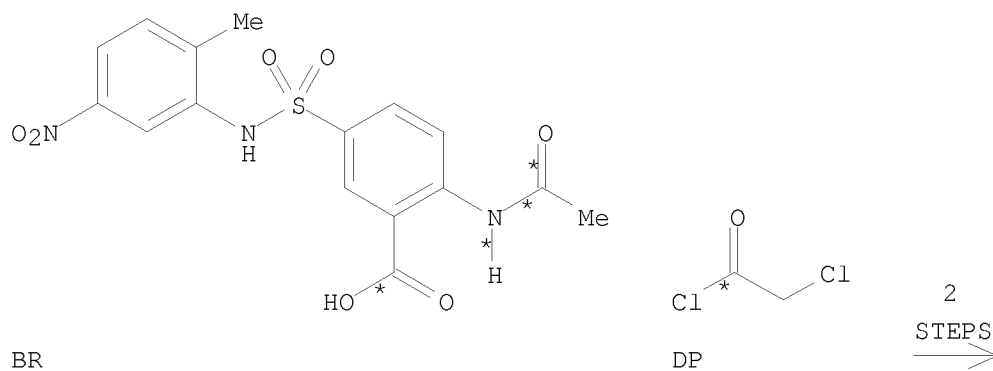
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EV 774217-91-3

RX(220) OF 372 COMPOSED OF RX(71), RX(108)  
RX(220) BR + DP ==> EW



EW  
YIELD 58%

RX(71) RCT BR 774217-17-3

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH

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CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DK 774217-54-8

NTE chemoselective

RX(108) RCT DK 774217-54-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

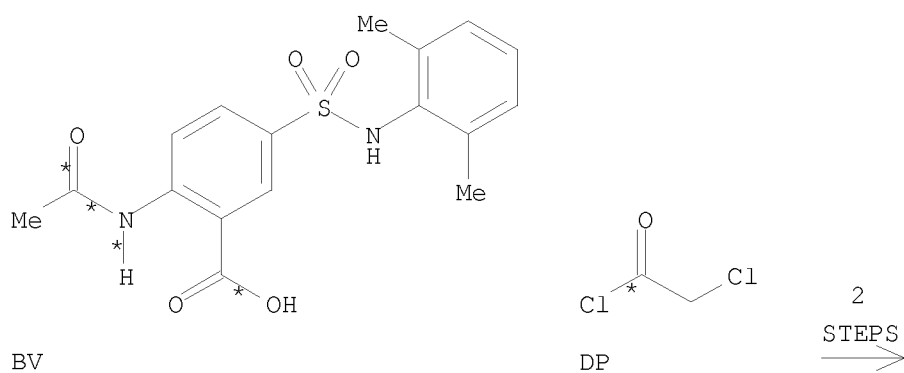
RGT D 7732-18-5 Water

CON cooled

PRO EW 774217-92-4

RX(221) OF 372 COMPOSED OF RX(72), RX(109)

RX(221) BV + DP ==> EX



EX  
YIELD 56%

RX(72) RCT BV 774217-19-5

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STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DL 774217-56-0  
NTE chemoselective

RX(109) RCT DL 774217-56-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

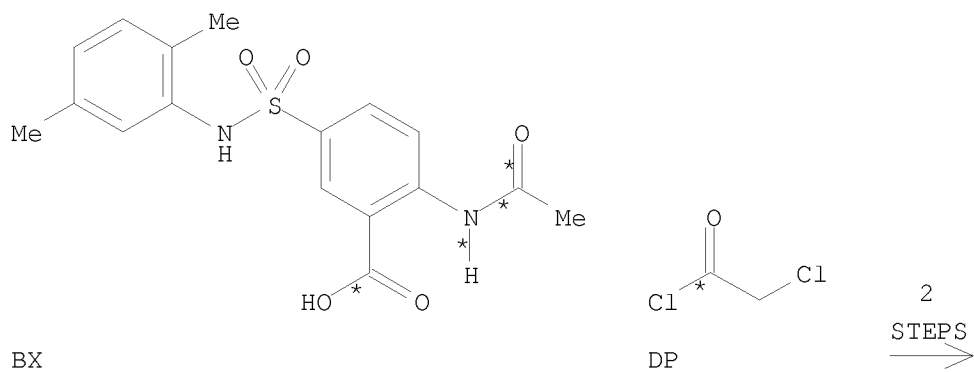
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EX 774217-94-6

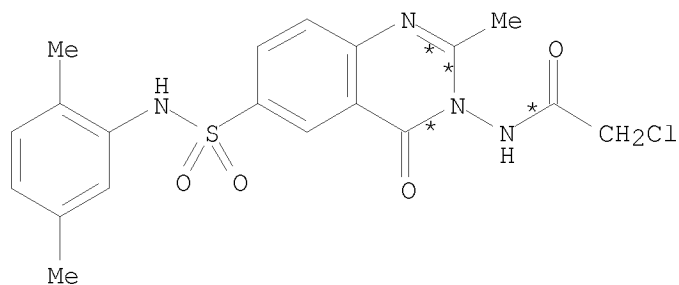
RX(222) OF 372 COMPOSED OF RX(73), RX(110)

RX(222) BX + DP ==> EY





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EY  
YIELD 59%

RX(73) RCT BX 774217-20-8

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DM 774217-57-1

NTE chemoselective

RX(110) RCT DM 774217-57-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

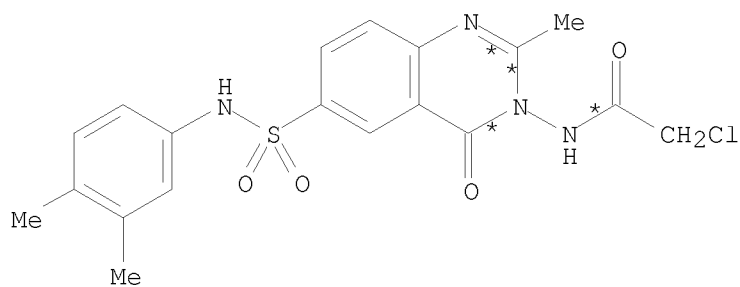
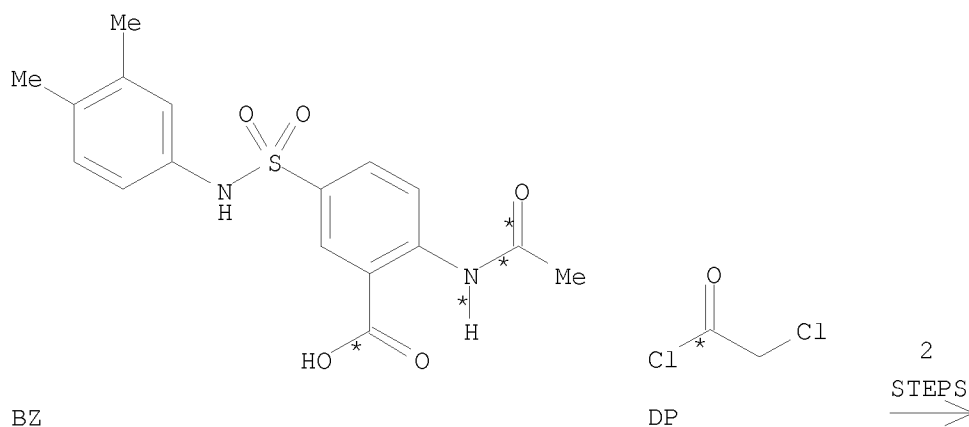
CON cooled

PRO EY 774217-95-7

RX(223) OF 372 COMPOSED OF RX(74), RX(111)

RX(223) BZ + DP ==> EZ

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EZ  
YIELD 62%

RX(74) RCT BZ 774217-21-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DN 774217-58-2  
NTE chemoselective

RX(111) RCT DN 774217-58-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

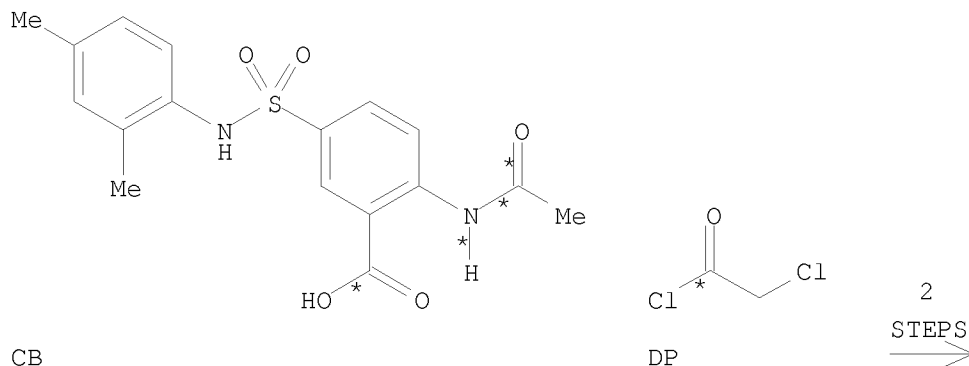
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CON cooled

PRO EZ 774217-96-8

RX(224) OF 372 COMPOSED OF RX(75), RX(112)

RX(224) CB + DP ==> FA



FA  
YIELD 70%

RX(75) RCT CB 774217-22-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DO 774217-59-3

NTE chemoselective

RX(112) RCT DO 774217-59-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

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STAGE(2)

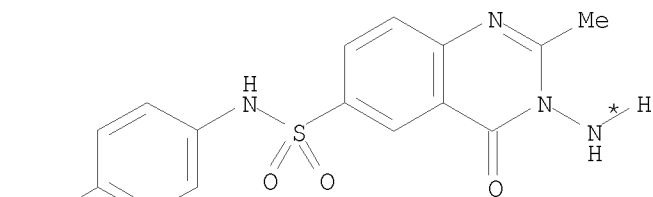
RGT D 7732-18-5 Water

CON cooled

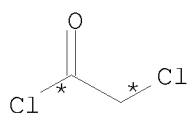
PRO FA 774217-97-9

RX(249) OF 372 COMPOSED OF RX(100), RX(137)

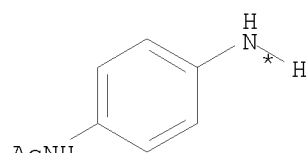
RX(249) DC + DP + BA ==> FZ



DC

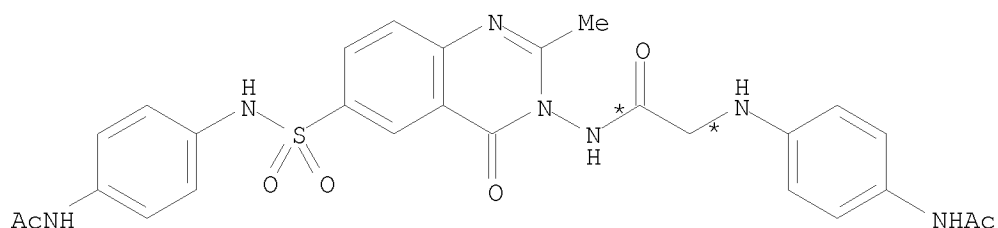


DP



BA

2  
STEPS  
→



FZ

YIELD 53%

RX(100) RCT DC 774217-46-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

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CON cooled

PRO EO 774217-84-4

RX(137) RCT BA 122-80-5, EO 774217-84-4

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

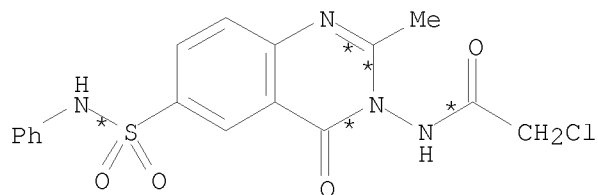
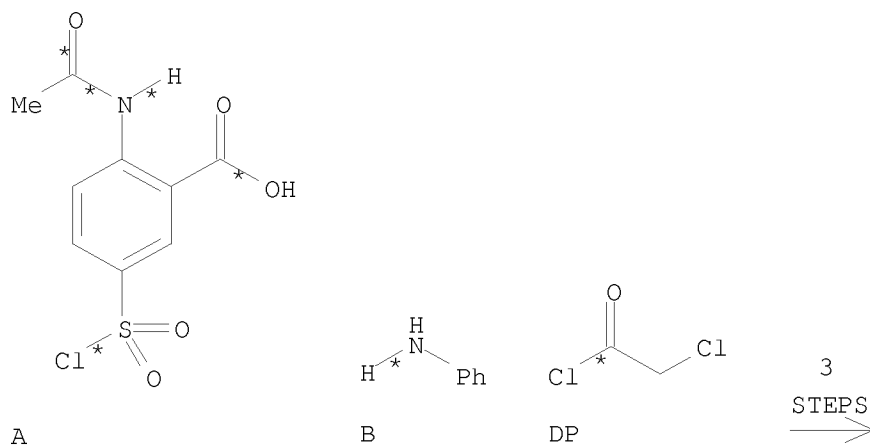
RGT D 7732-18-5 Water

CON cooled

PRO FZ 774218-18-7

RX(262) OF 372 COMPOSED OF RX(1), RX(39), RX(76)

RX(262) A + B + DP ==> DQ



DQ  
YIELD 61%

RX(1) RCT A 181478-44-4, B 62-53-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

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CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO C 774216-86-3

RX(39) RCT C 774216-86-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CC 774217-23-1  
NTE chemoselective

RX(76) RCT CC 774217-23-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

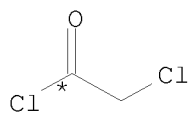
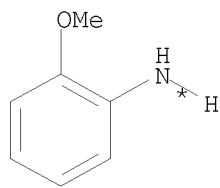
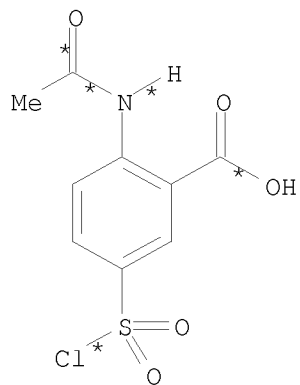
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DQ 774217-60-6

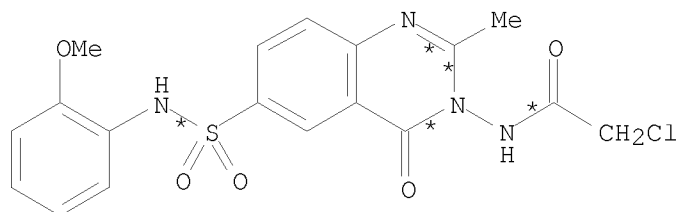
RX(263) OF 372 COMPOSED OF RX(2), RX(40), RX(77)

RX(263) A + G + DP ==> DR



3  
STEPS  
→

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DR  
YIELD 59%

RX(2) RCT A 181478-44-4, G 90-04-0

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO H 774216-87-4

RX(40) RCT H 774216-87-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CF 774217-24-2

NTE chemoselective

RX(77) RCT CF 774217-24-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

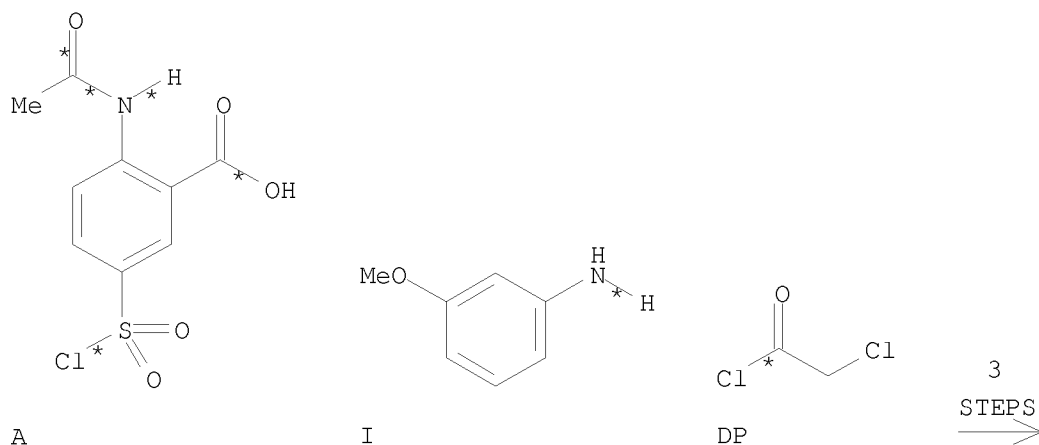
CON cooled

PRO DR 774217-61-7

RX(264) OF 372 COMPOSED OF RX(3), RX(41), RX(78)

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RX(264)    A   +   I   +   DP   ==>   DS



DS  
YIELD 53%

RX(3)        RCT   A 181478-44-4, I 536-90-3

STAGE(1)

CAT   110-86-1 Pyridine

SOL   64-17-5 EtOH

CON   SUBSTAGE(1) 4 hours, 120 deg C

         SUBSTAGE(2) cooled

STAGE(2)

RGT   D 7732-18-5 Water

CON   cooled

PRO   J 774216-88-5

RX(41)       RCT   J 774216-88-5

STAGE(1)

RGT   CD 7803-57-8 N2H4-H2O

SOL   67-56-1 MeOH

CON   3 hours, reflux

STAGE(2)

RGT   D 7732-18-5 Water



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CON cooled

PRO CG 774217-25-3

NTE chemoselective

RX(78) RCT CG 774217-25-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

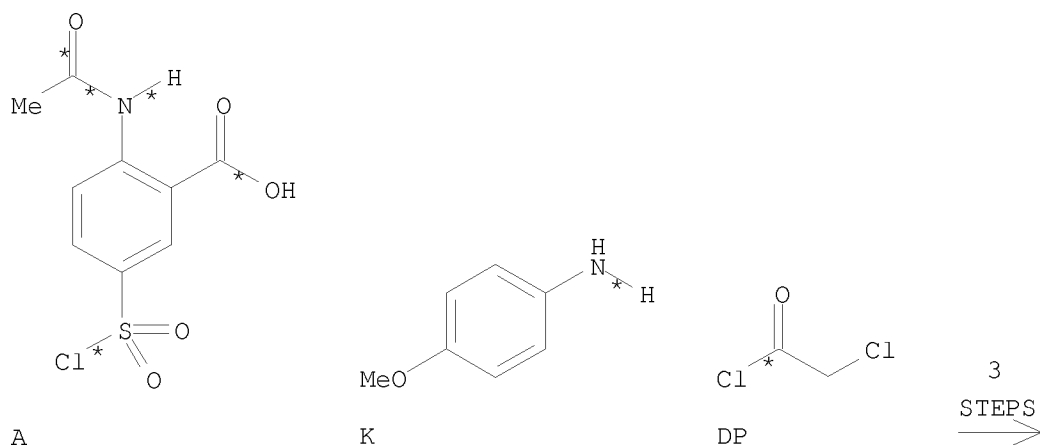
RGT D 7732-18-5 Water

CON cooled

PRO DS 774217-62-8

RX(265) OF 372 COMPOSED OF RX(4), RX(42), RX(79)

RX(265) A + K + DP ==> DT



DT  
YIELD 63%

RX(4) RCT A 181478-44-4, K 104-94-9

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STAGE(1)  
CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO L 774216-89-6

RX(42) RCT L 774216-89-6

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CH 774217-26-4  
NTE chemoselective

RX(79) RCT CH 774217-26-4, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

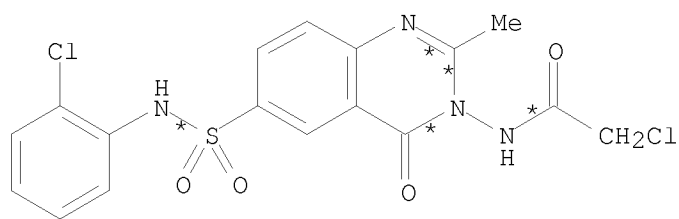
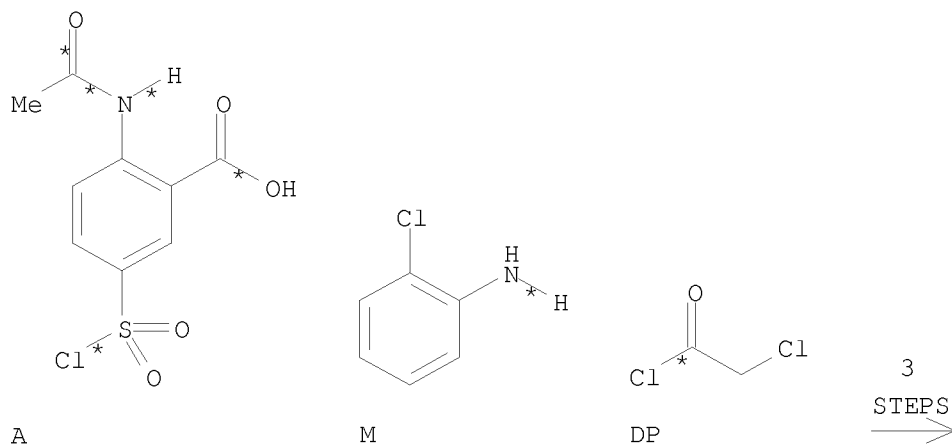
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DT 774217-63-9

RX(266) OF 372 COMPOSED OF RX(5), RX(43), RX(80)

RX(266) A + M + DP ==> DU

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DU  
YIELD 53%

RX(5) RCT A 181478-44-4, M 95-51-2

STAGE(1)

CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO N 774216-90-9

RX(43) RCT N 774216-90-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

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PRO CI 774217-27-5  
NTE chemoselective

RX(80) RCT CI 774217-27-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

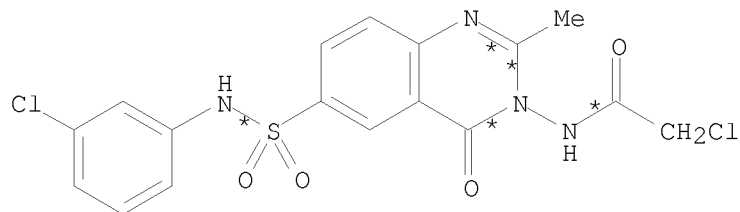
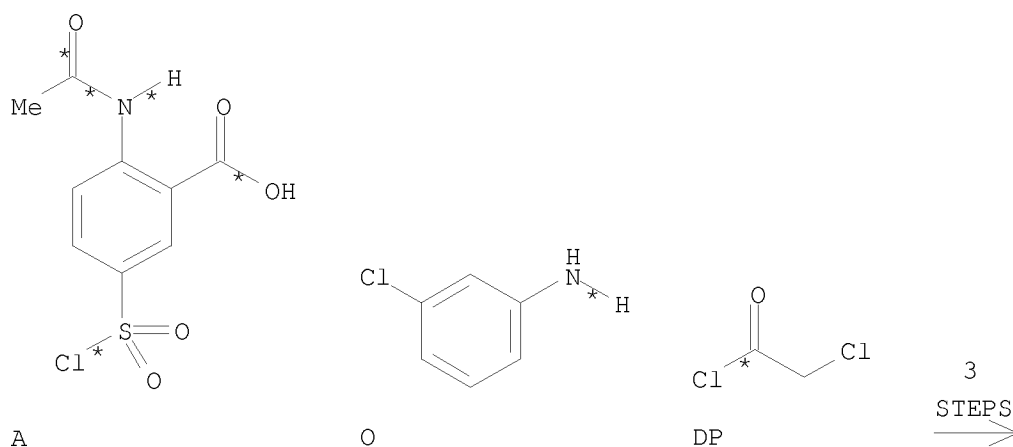
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DU 774217-64-0

RX(267) OF 372 COMPOSED OF RX(6), RX(44), RX(81)

RX(267) A + O + DP ==> DV



DV  
YIELD 59%

RX(6) RCT A 181478-44-4, O 108-42-9

STAGE(1)

CAT 110-86-1 Pyridine

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SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO P 774216-91-0

RX(44) RCT P 774216-91-0

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CJ 774217-28-6  
NTE chemoselective

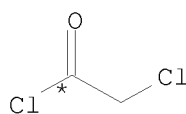
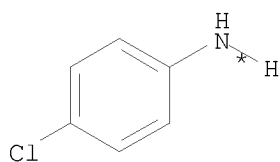
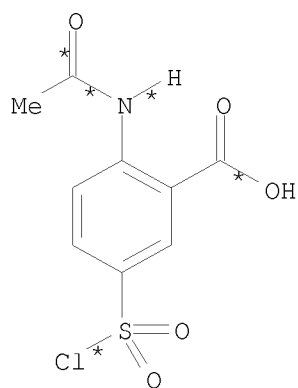
RX(81) RCT CJ 774217-28-6, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

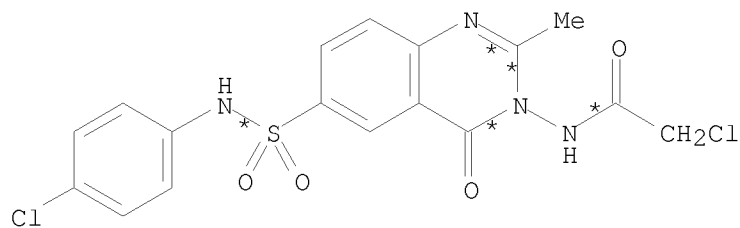
PRO DV 774217-65-1

RX(268) OF 372 COMPOSED OF RX(7), RX(45), RX(82)  
RX(268) A + Q + DP ==> DW



3  
STEPS  
→

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DW  
YIELD 58%

RX(7) RCT A 181478-44-4, Q 106-47-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO R 774216-92-1

RX(45) RCT R 774216-92-1

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CK 774217-29-7

NTE chemoselective

RX(82) RCT CK 774217-29-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

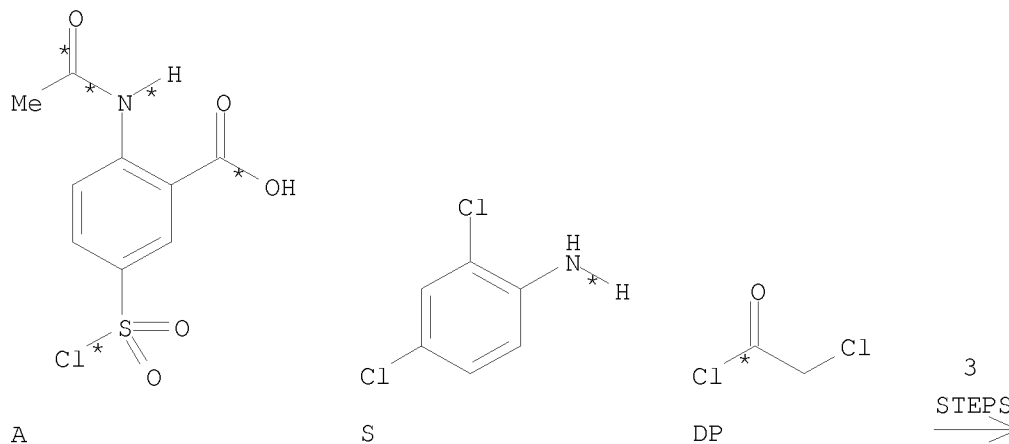
RGT D 7732-18-5 Water

CON cooled

PRO DW 774217-66-2

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RX(269) OF 372 COMPOSED OF RX(8), RX(46), RX(83)  
RX(269) A + S + DP ==> DX



DX  
YIELD 63%

RX(8) RCT A 181478-44-4, S 554-00-7

STAGE(1)

CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO T 774216-93-2

RX(46) RCT T 774216-93-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

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RGT D 7732-18-5 Water  
CON cooled

PRO CL 774217-30-0  
NTE chemoselective

RX(83) RCT CL 774217-30-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

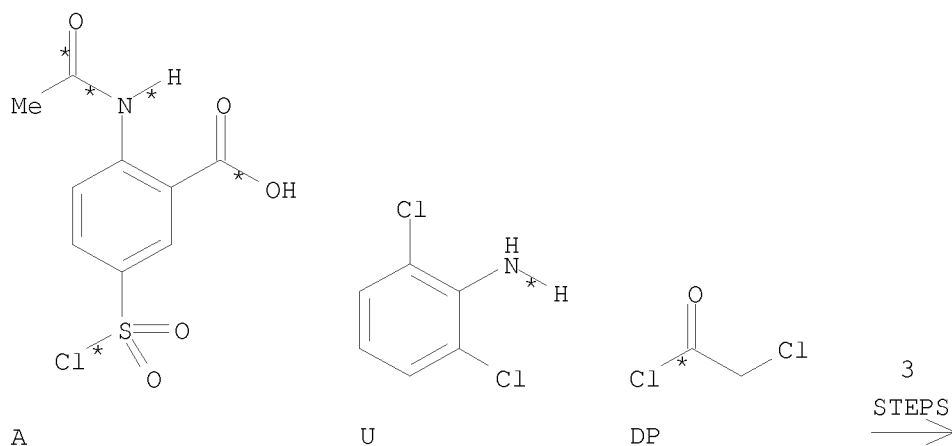
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DX 774217-67-3

RX(270) OF 372 COMPOSED OF RX(9), RX(47), RX(84)

RX(270) A + U + DP ==> DY



DY  
YIELD 57%

RX(9) RCT A 181478-44-4, U 608-31-1



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STAGE(1)  
CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO V 774216-94-3

RX(47) RCT V 774216-94-3

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CM 774217-31-1  
NTE chemoselective

RX(84) RCT CM 774217-31-1, DP 79-04-9

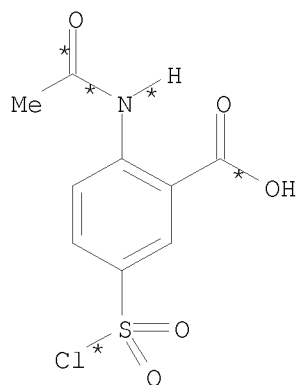
STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

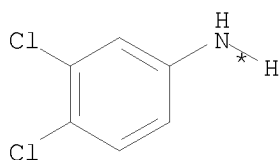
PRO DY 774217-68-4

RX(271) OF 372 COMPOSED OF RX(10), RX(48), RX(85)  
RX(271) A + W + DP ==> DZ

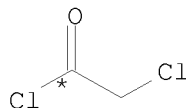
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A

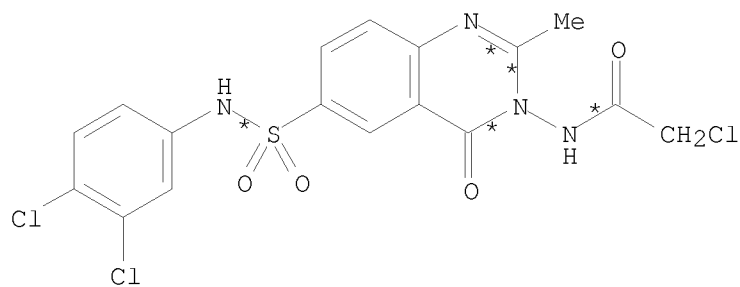


W



DP

3  
STEPS  
→



DZ  
YIELD 57%

RX(10) RCT A 181478-44-4, W 95-76-1

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO X 774216-95-4

RX(48) RCT X 774216-95-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

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CON cooled

PRO CN 774217-32-2

NTE chemoselective

RX(85) RCT CN 774217-32-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

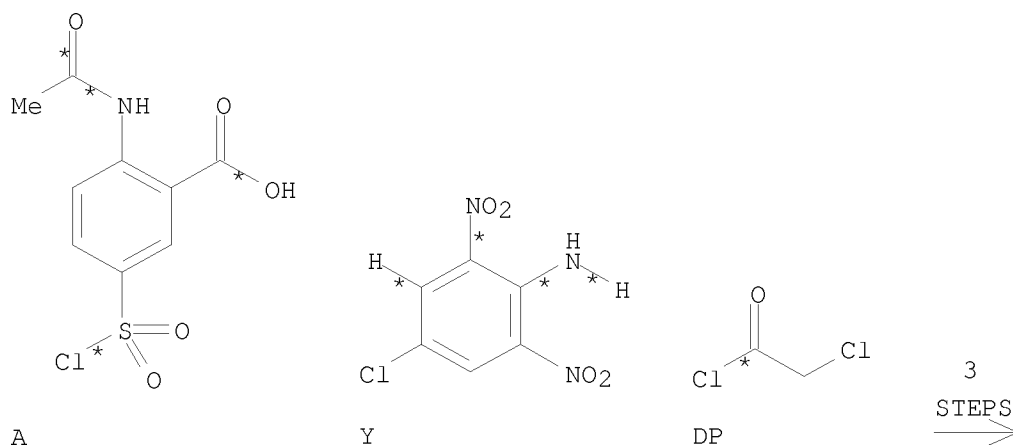
RGT D 7732-18-5 Water

CON cooled

PRO DZ 774217-69-5

RX(272) OF 372 COMPOSED OF RX(11), RX(49), RX(86)

RX(272) A + Y + DP ==> EA



EA  
YIELD 62%

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RX(11) RCT A 181478-44-4, Y 5388-62-5

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO Z 218617-81-3

RX(49) RCT Z 218617-81-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CO 234096-58-3

NTE chemoselective

RX(86) RCT CO 234096-58-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

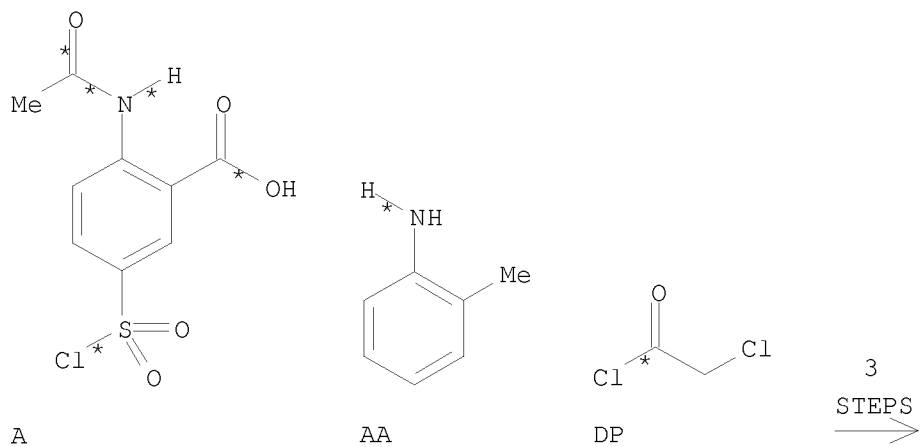
CON cooled

PRO EA 774217-70-8

RX(273) OF 372 COMPOSED OF RX(12), RX(50), RX(87)

RX(273) A + AA + DP ==> EB

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EB  
YIELD 59%

RX(12) RCT A 181478-44-4, AA 95-53-4

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AB 774216-96-5

RX(50) RCT AB 774216-96-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

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PRO CP 774217-33-3  
NTE chemoselective

RX(87) RCT CP 774217-33-3, DP 79-04-9

STAGE(1)

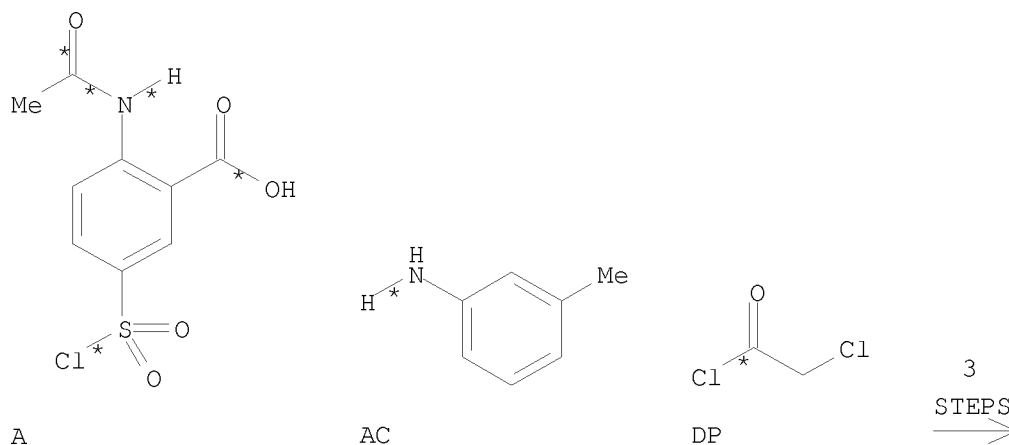
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EB 774217-71-9

RX(274) OF 372 COMPOSED OF RX(13), RX(51), RX(88)  
RX(274) A + AC + DP ==> EC



EC  
YIELD 64%

RX(13) RCT A 181478-44-4, AC 108-44-1

STAGE(1)

CAT 110-86-1 Pyridine

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SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO AD 774216-97-6

RX(51) RCT AD 774216-97-6

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CQ 774217-34-4  
NTE chemoselective

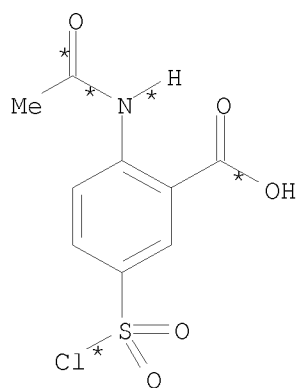
RX(88) RCT CQ 774217-34-4, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

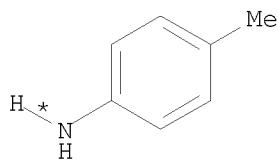
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EC 774217-72-0

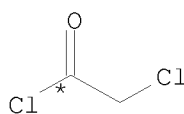
RX(275) OF 372 COMPOSED OF RX(14), RX(52), RX(89)  
RX(275) A + AE + DP ==> ED



A



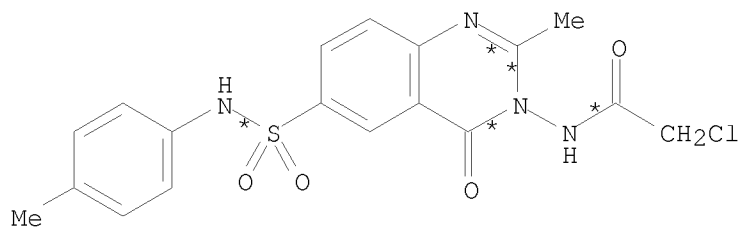
AE



DP

3  
STEPS  
→

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ED  
YIELD 63%

RX(14) RCT A 181478-44-4, AE 106-49-0

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AF 774216-98-7

RX(52) RCT AF 774216-98-7

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CR 774217-35-5

NTE chemoselective

RX(89) RCT CR 774217-35-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

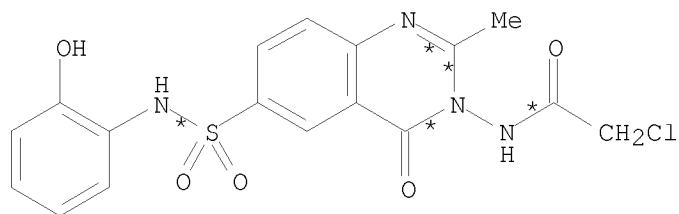
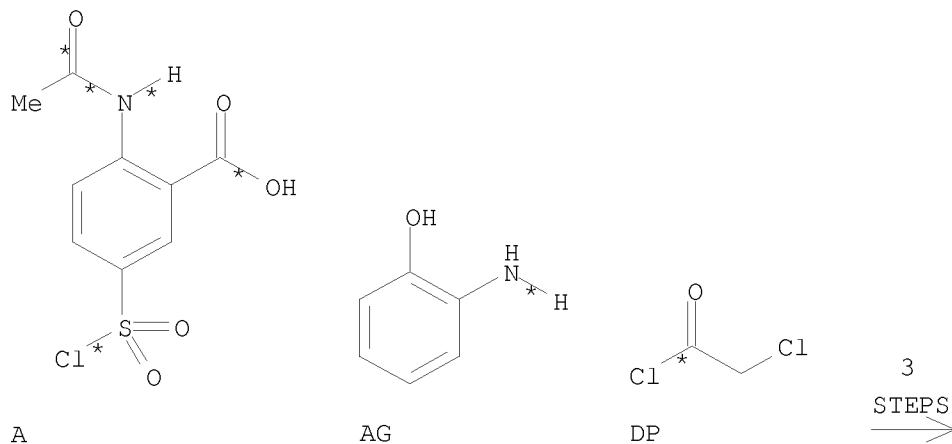
CON cooled

PRO ED 774217-73-1



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RX(276) OF 372 COMPOSED OF RX(15), RX(53), RX(90)  
RX(276) A + AG + DP ==> EE



EE  
YIELD 58%

RX(15) RCT A 181478-44-4, AG 95-55-6

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AH 774216-99-8

RX(53) RCT AH 774216-99-8

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

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RGT D 7732-18-5 Water  
CON cooled

PRO CS 774217-36-6  
NTE chemoselective

RX(90) RCT CS 774217-36-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

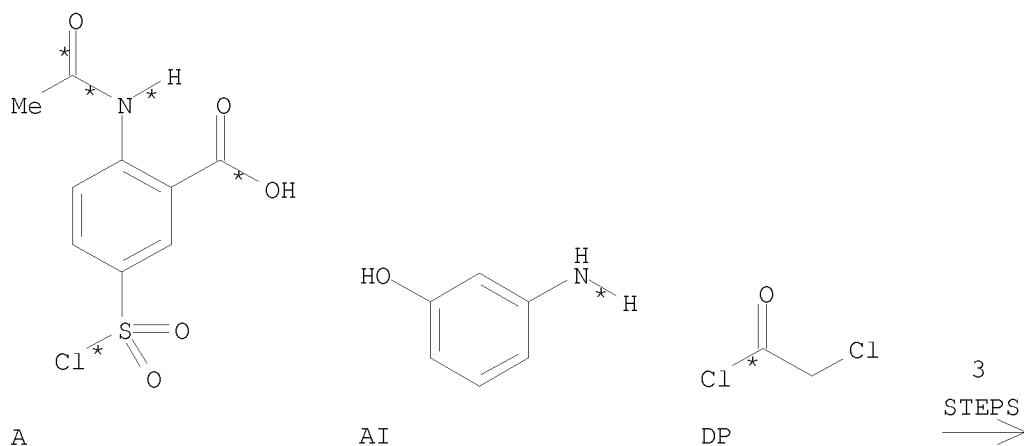
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EE 774217-74-2

RX(277) OF 372 COMPOSED OF RX(16), RX(54), RX(91)

RX(277) A + AI + DP ==> EF



EF  
YIELD 59%

RX(16) RCT A 181478-44-4, AI 591-27-5

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STAGE(1)  
CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO AJ 774217-00-4

RX(54) RCT AJ 774217-00-4

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CT 774217-37-7  
NTE chemoselective

RX(91) RCT CT 774217-37-7, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

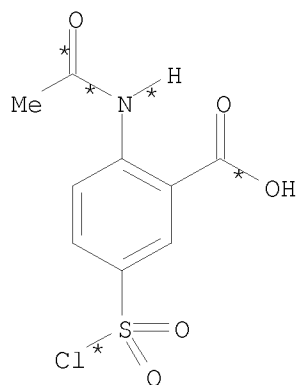
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EF 774217-75-3

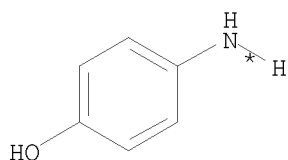
RX(278) OF 372 COMPOSED OF RX(17), RX(55), RX(92)

RX(278) A + AK + DP ==> EG

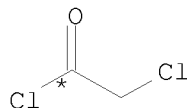
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A

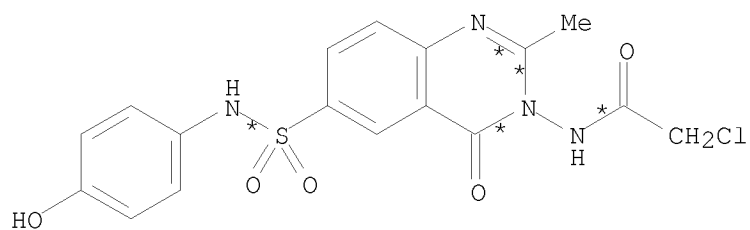


AK



DP

3  
STEPS  
→



EG  
YIELD 63%

RX(17) RCT A 181478-44-4, AK 123-30-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AL 774217-01-5

RX(55) RCT AL 774217-01-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

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PRO CU 774217-38-8  
NTE chemoselective

RX(92) RCT CU 774217-38-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

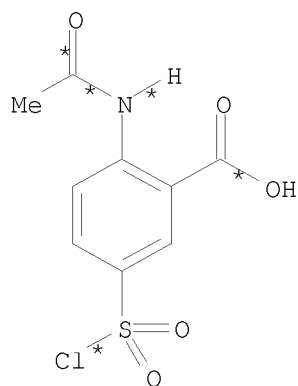
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

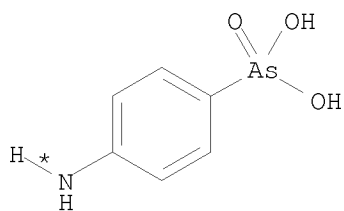
PRO EG 774217-76-4

RX(279) OF 372 COMPOSED OF RX(18), RX(56), RX(93)

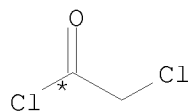
RX(279) A + AM + DP ==> EH



A

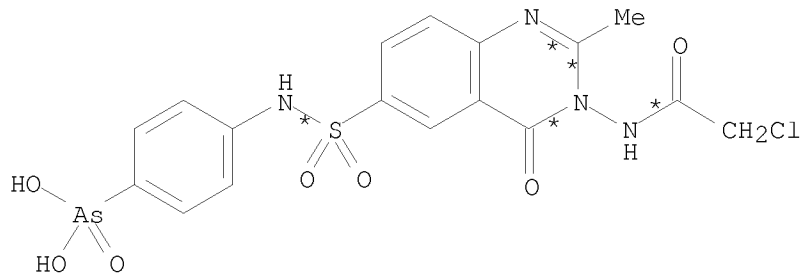


AM



DP

3  
STEPS  
→



EH  
YIELD 71%

RX(18) RCT A 181478-44-4, AM 98-50-0

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STAGE(1)  
CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO AN 774217-02-6

RX(56) RCT AN 774217-02-6

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CV 774217-39-9  
NTE chemoselective

RX(93) RCT CV 774217-39-9, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

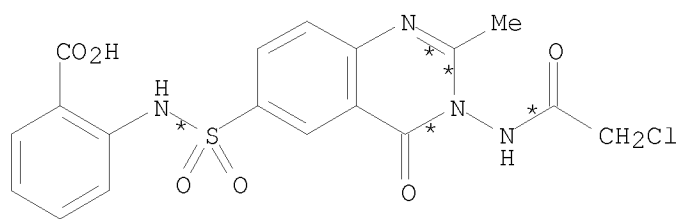
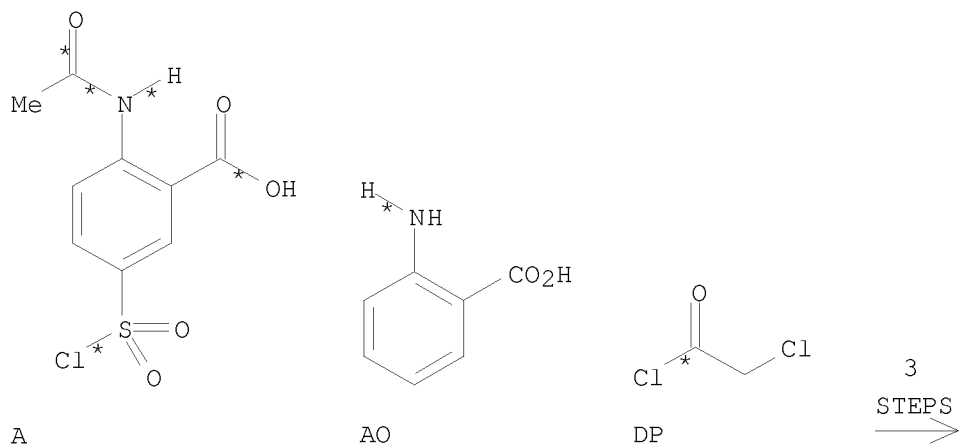
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EH 774217-77-5

RX(280) OF 372 COMPOSED OF RX(19), RX(57), RX(94)

RX(280) A + AO + DP ==> EI

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EI  
YIELD 75%

RX(19) RCT A 181478-44-4, AO 118-92-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AP 774217-03-7

RX(57) RCT AP 774217-03-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

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PRO CW 774217-40-2  
NTE chemoselective

RX(94) RCT CW 774217-40-2, DP 79-04-9

STAGE (1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE (2) cooled

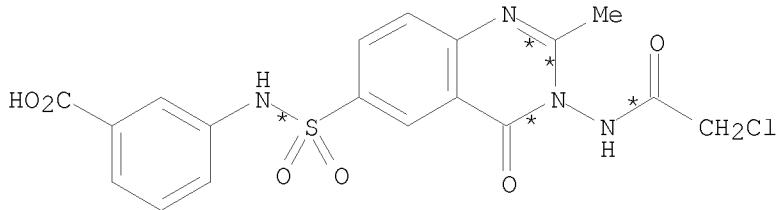
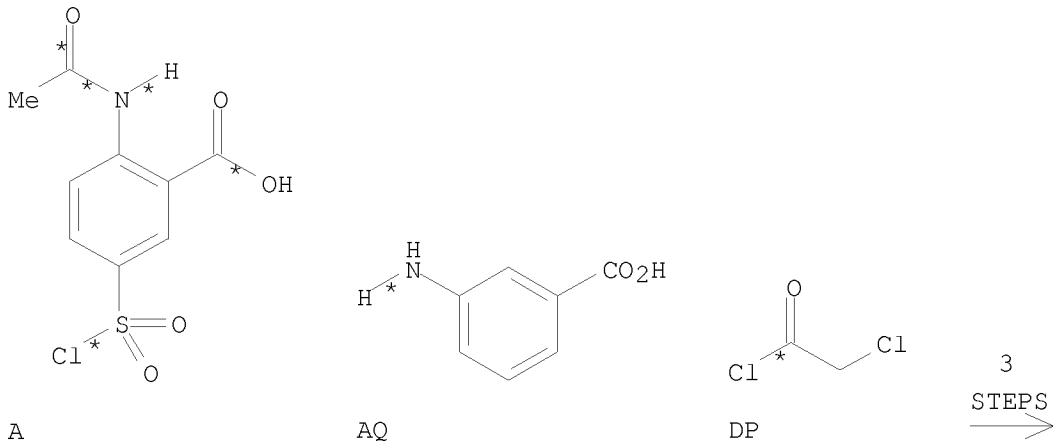
STAGE (2)

RGT D 7732-18-5 Water

CON    cooled

PRO EI 774217-78-6

RX(281) OF 372 COMPOSED OF RX(20), RX(58), RX(95)

$$\text{RX}(281) \quad \text{A} \quad + \quad \text{AQ} \quad + \quad \text{DP} \quad ==\Rightarrow \quad \text{EJ}$$


EJ  
YIELD 70%

RX(20) RCT A 181478-44-4, AQ 99-05-8

STAGE (1)

CAT 110-86-1 Pyridine



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SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO AR 774217-04-8

RX(58) RCT AR 774217-04-8

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CX 774217-41-3  
NTE chemoselective

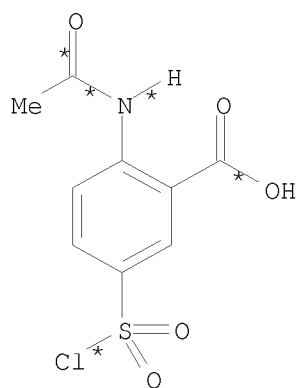
RX(95) RCT CX 774217-41-3, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

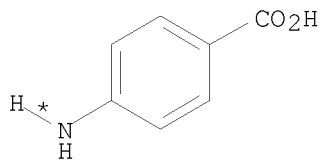
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EJ 774217-79-7

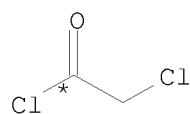
RX(282) OF 372 COMPOSED OF RX(21), RX(59), RX(96)  
RX(282) A + AS + DP ==> EK



A



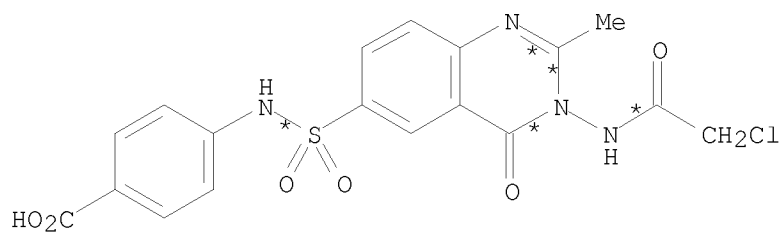
AS



DP

3  
STEPS  
→

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EK  
YIELD 68%

RX(21) RCT A 181478-44-4, AS 150-13-0

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AT 774217-05-9

RX(59) RCT AT 774217-05-9

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CY 774217-42-4

NTE chemoselective

RX(96) RCT CY 774217-42-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

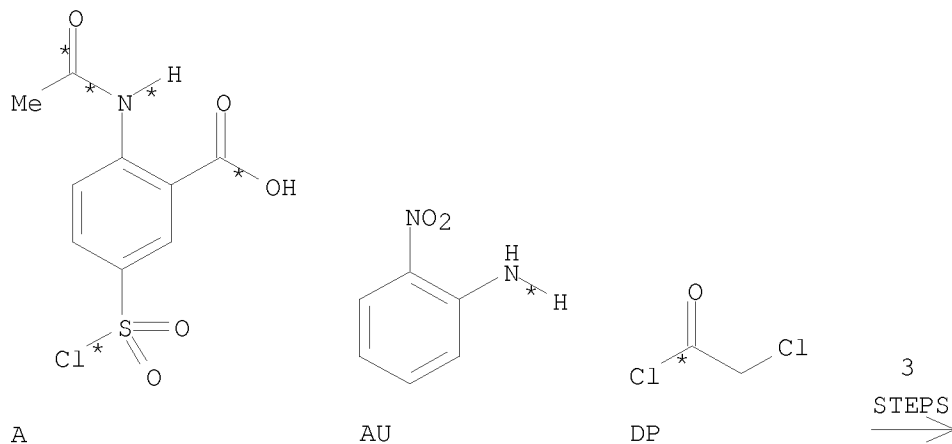
RGT D 7732-18-5 Water

CON cooled

PRO EK 774217-80-0

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RX(283) OF 372 COMPOSED OF RX(22), RX(60), RX(97)  
RX(283) A + AU + DP ==> EL



EL  
YIELD 75%

RX(22) RCT A 181478-44-4, AU 88-74-4

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AV 774217-06-0

RX(60) RCT AV 774217-06-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

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RGT D 7732-18-5 Water  
CON cooled

PRO CZ 774217-43-5  
NTE chemoselective

RX(97) RCT CZ 774217-43-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

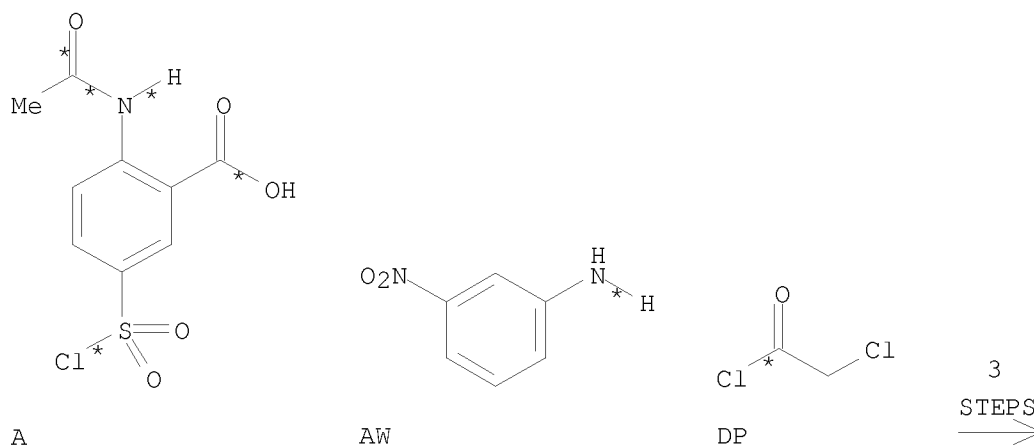
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EL 774217-81-1

RX(284) OF 372 COMPOSED OF RX(23), RX(61), RX(98)

RX(284) A + AW + DP ==> EM



EM  
YIELD 78%

RX(23) RCT A 181478-44-4, AW 99-09-2

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STAGE(1)  
CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO AX 774217-07-1

RX(61) RCT AX 774217-07-1

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DA 774217-44-6  
NTE chemoselective

RX(98) RCT DA 774217-44-6, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

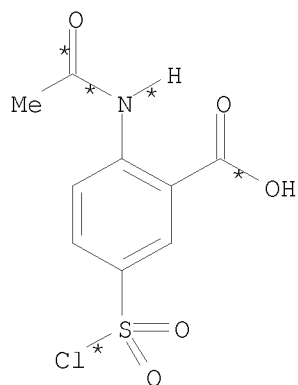
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EM 774217-82-2

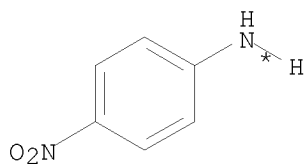
RX(285) OF 372 COMPOSED OF RX(24), RX(62), RX(99)

RX(285) A + AY + DP ==> EN

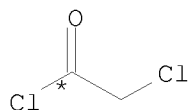
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A

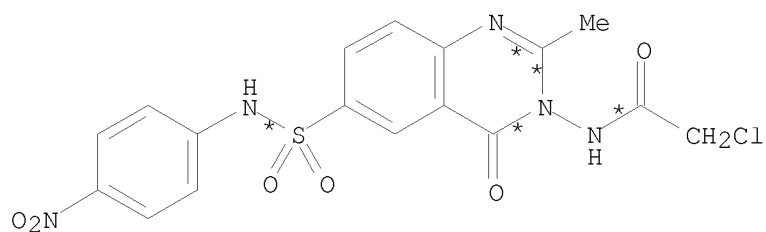


AY



DP

3  
STEPS  
→



EN  
YIELD 71%

RX(24) RCT A 181478-44-4, AY 100-01-6

STAGE(1)

CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO AZ 774217-08-2

RX(62) RCT AZ 774217-08-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

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PRO DB 774217-45-7  
NTE chemoselective

RX(99) RCT DB 774217-45-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

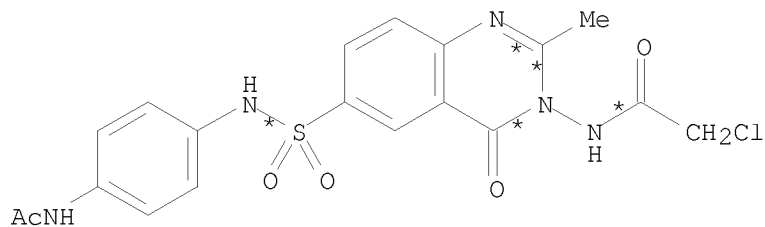
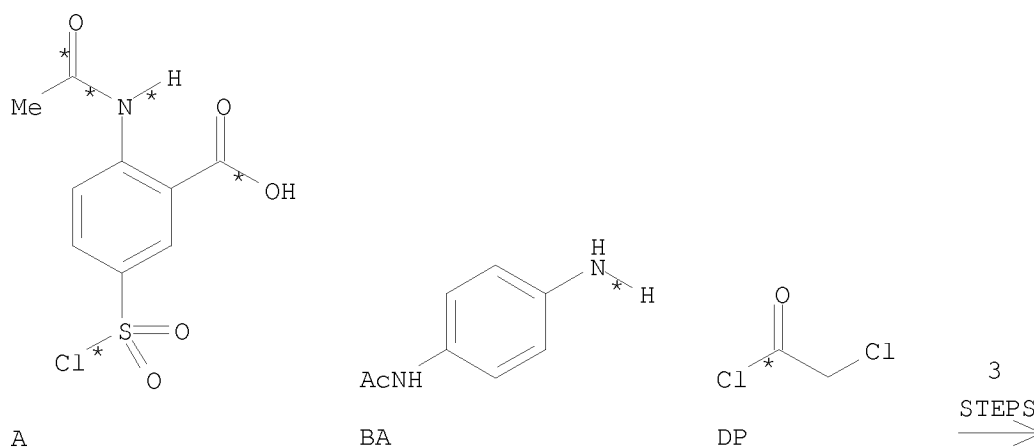
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EN 774217-83-3

RX(286) OF 372 COMPOSED OF RX(25), RX(63), RX(100)

RX(286) A + BA + DP ==> EO



EO  
YIELD 53%

RX(25) RCT A 181478-44-4, BA 122-80-5

STAGE(1)

CAT 110-86-1 Pyridine

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SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO BB 774217-09-3

RX(63) RCT BB 774217-09-3

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DC 774217-46-8  
NTE chemoselective

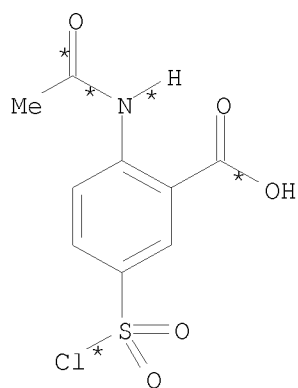
RX(100) RCT DC 774217-46-8, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

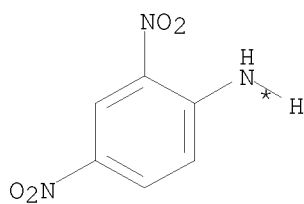
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EO 774217-84-4

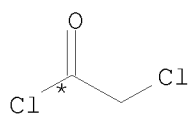
RX(287) OF 372 COMPOSED OF RX(26), RX(64), RX(101)  
RX(287) A + BC + DP ==> EP



A



BC

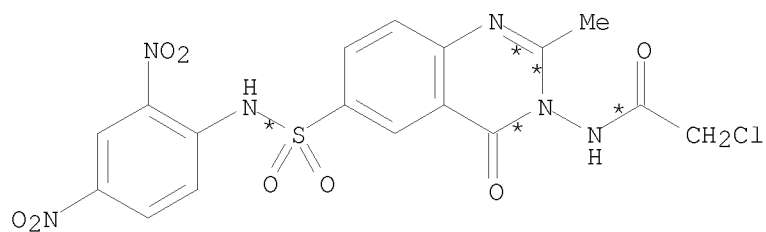


DP

3  
STEPS  
→



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EP  
YIELD 57%

RX(26) RCT A 181478-44-4, BC 97-02-9

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BD 774217-10-6

RX(64) RCT BD 774217-10-6

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DD 774217-47-9

NTE chemoselective

RX(101) RCT DD 774217-47-9, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

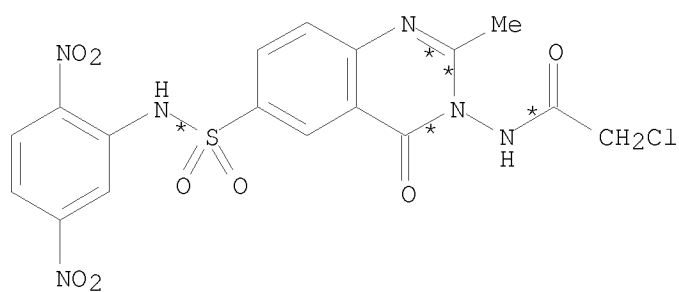
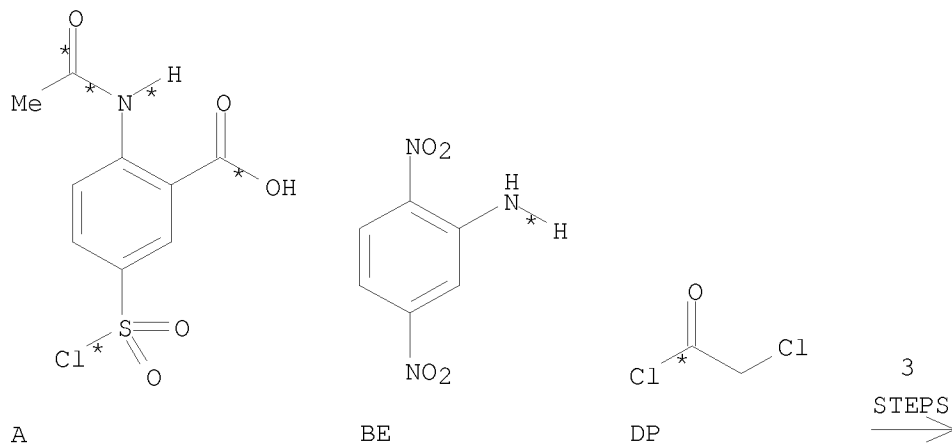
RGT D 7732-18-5 Water

CON cooled

PRO EP 774217-85-5

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RX(288) OF 372 COMPOSED OF RX(27), RX(65), RX(102)  
RX(288) A + BE + DP ==> EQ



EQ  
YIELD 57%

RX(27) RCT A 181478-44-4, BE 619-18-1

STAGE(1)  
CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO BF 774217-11-7

RX(65) RCT BF 774217-11-7

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

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STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DE 774217-48-0  
NTE chemoselective

RX(102) RCT DE 774217-48-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

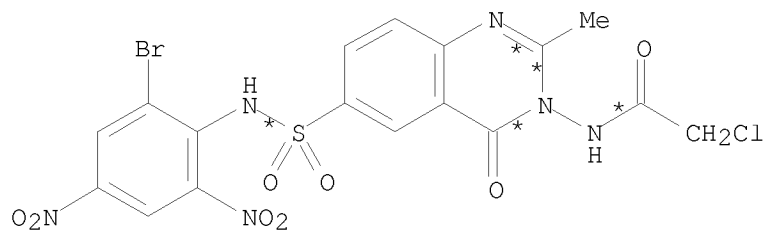
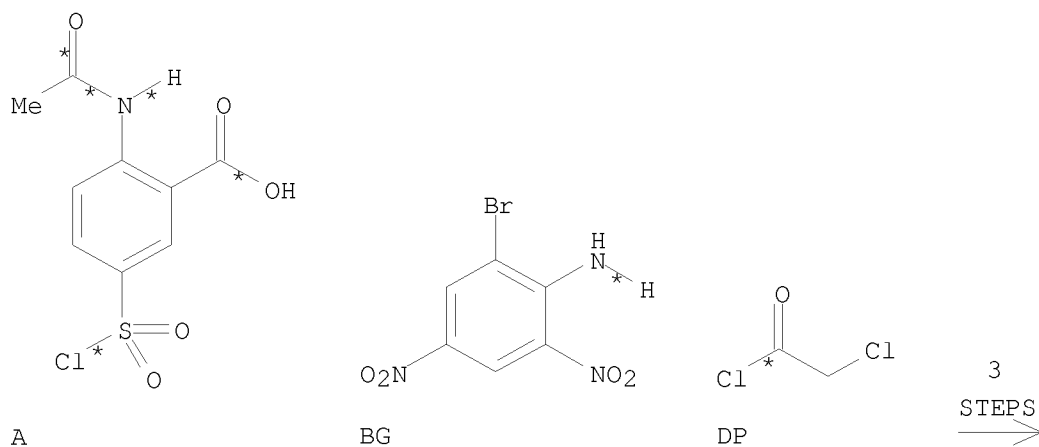
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EQ 774217-86-6

RX(289) OF 372 COMPOSED OF RX(28), RX(66), RX(103)

RX(289) A + BG + DP ==> ER



ER  
YIELD 54%

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RX(28) RCT A 181478-44-4, BG 1817-73-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BH 774217-12-8

RX(66) RCT BH 774217-12-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DF 774217-49-1

NTE chemoselective

RX(103) RCT DF 774217-49-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

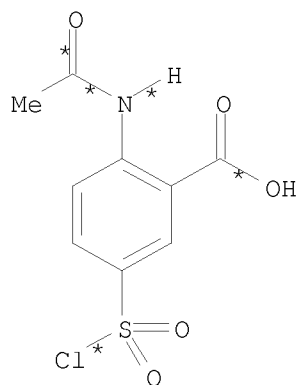
CON cooled

PRO ER 774217-87-7

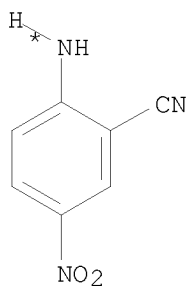
RX(290) OF 372 COMPOSED OF RX(29), RX(67), RX(104)

RX(290) A + BI + DP ==> ES

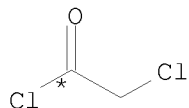
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A

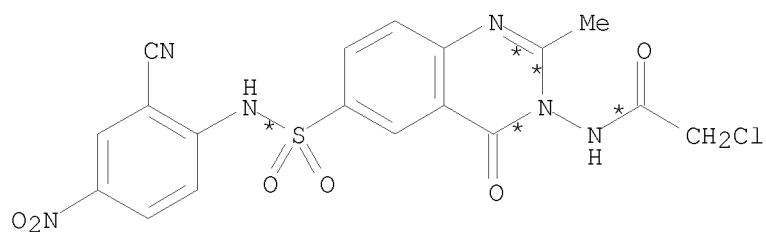


BI



DP

3  
STEPS  
→



ES  
YIELD 51%

RX(29) RCT A 181478-44-4, BI 17420-30-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BJ 774217-13-9

RX(67) RCT BJ 774217-13-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

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PRO DG 774217-50-4  
NTE chemoselective

RX(104) RCT DG 774217-50-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

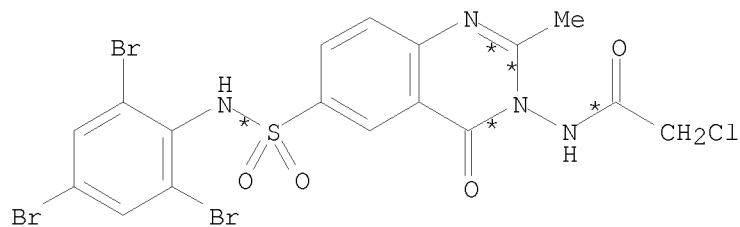
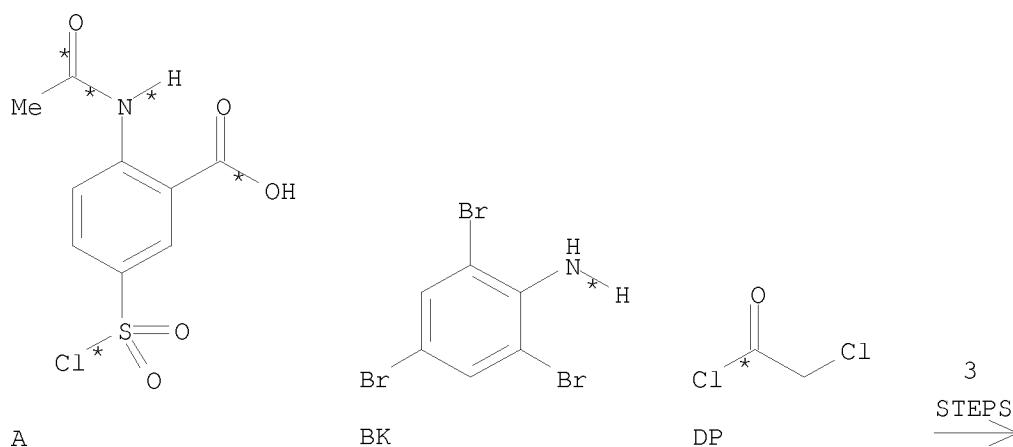
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO ES 774217-88-8

RX(291) OF 372 COMPOSED OF RX(30), RX(68), RX(105)

RX(291) A + BK + DP ==> ET



ET  
YIELD 58%

RX(30) RCT A 181478-44-4, BK 147-82-0

STAGE(1)

CAT 110-86-1 Pyridine

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SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO BL 774217-14-0

RX(68) RCT BL 774217-14-0

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DH 774217-51-5  
NTE chemoselective

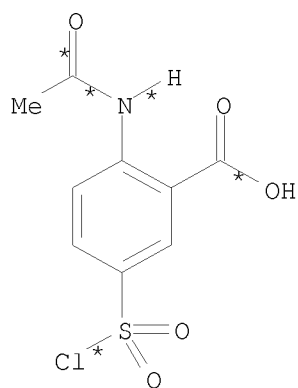
RX(105) RCT DH 774217-51-5, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

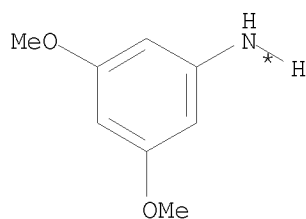
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO ET 774217-89-9

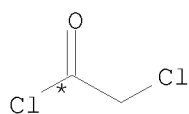
RX(292) OF 372 COMPOSED OF RX(31), RX(69), RX(106)  
RX(292) A + BM + DP ==> EU



A



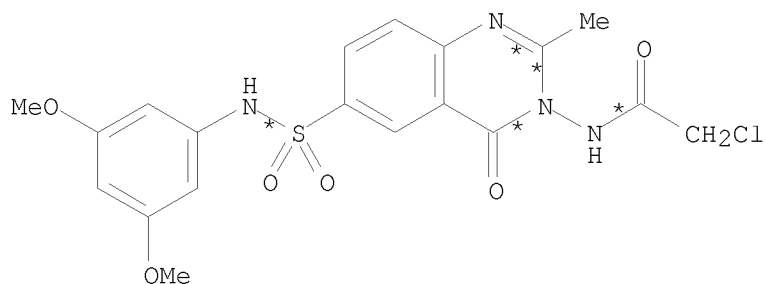
BM



DP

3  
STEPS  
→

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EU  
YIELD 63%

RX(31) RCT A 181478-44-4, BM 10272-07-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BN 774217-15-1

RX(69) RCT BN 774217-15-1

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DI 774217-52-6

NTE chemoselective

RX(106) RCT DI 774217-52-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

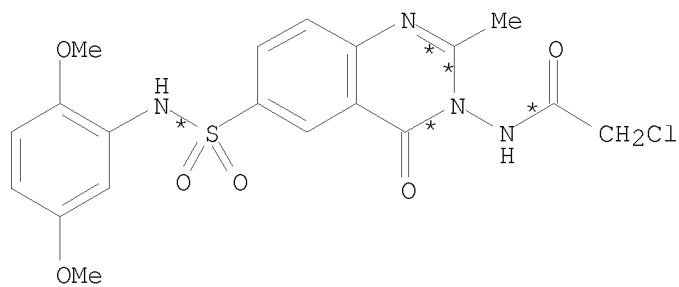
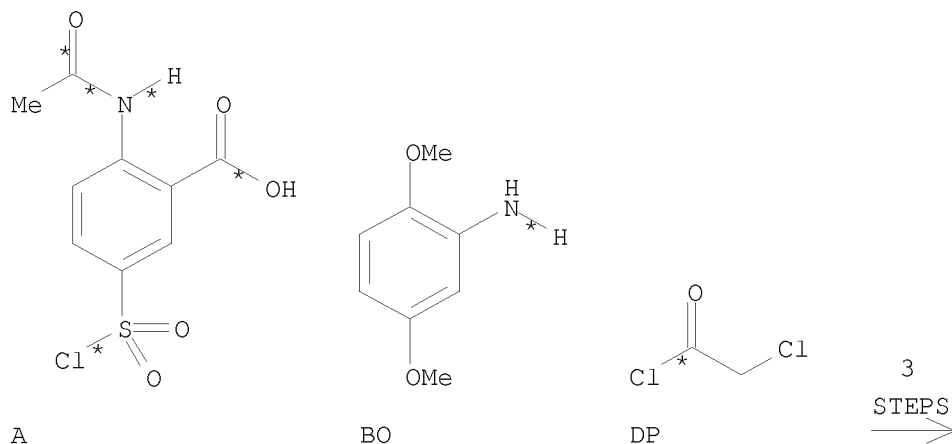
CON cooled

PRO EU 774217-90-2



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RX(293) OF 372 COMPOSED OF RX(32), RX(70), RX(107)  
RX(293) A + BO + DP ==> EV



EV  
YIELD 63%

RX(32) RCT A 181478-44-4, BO 102-56-7

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BP 774217-16-2

RX(70) RCT BP 774217-16-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

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SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DJ 774217-53-7  
NTE chemoselective

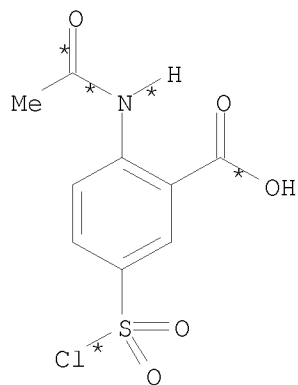
RX(107) RCT DJ 774217-53-7, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

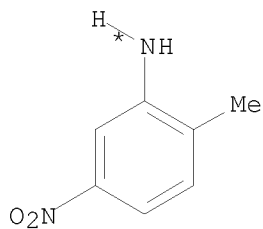
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EV 774217-91-3

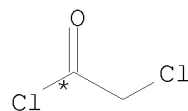
RX(294) OF 372 COMPOSED OF RX(33), RX(71), RX(108)  
RX(294) A + BQ + DP ==> EW



A



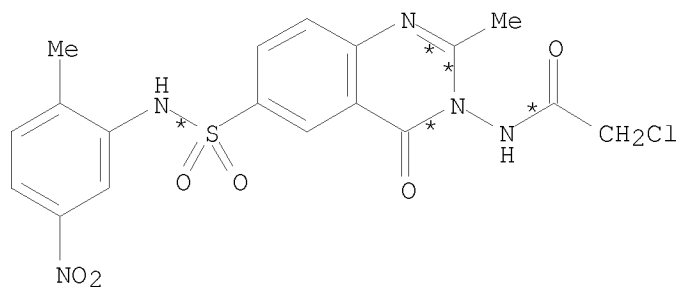
BQ



DP

3  
STEPS  
→

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EW  
YIELD 58%

RX(33) RCT A 181478-44-4, BQ 99-55-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BR 774217-17-3

RX(71) RCT BR 774217-17-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DK 774217-54-8

NTE chemoselective

RX(108) RCT DK 774217-54-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

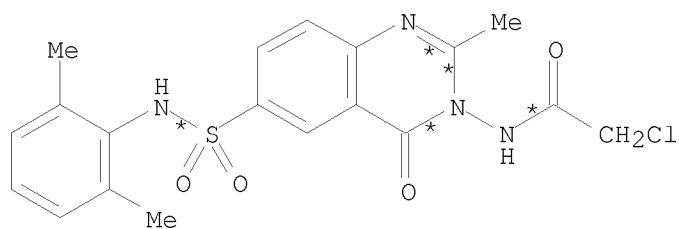
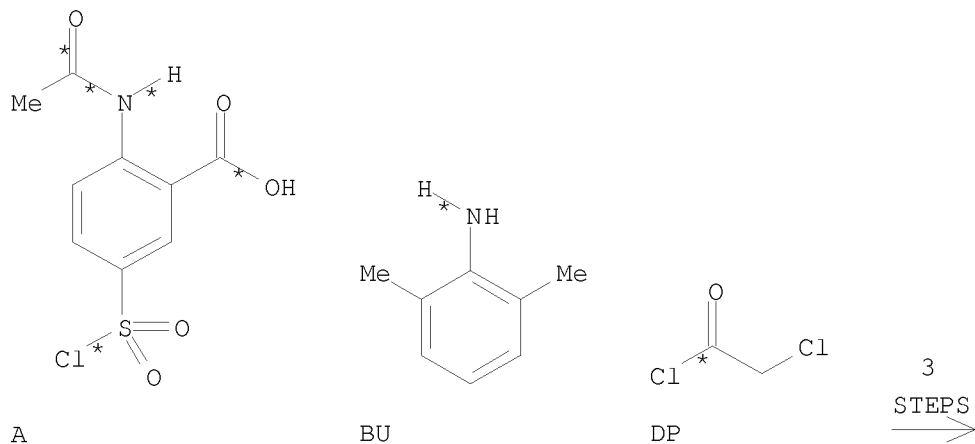
RGT D 7732-18-5 Water

CON cooled

PRO EW 774217-92-4

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RX(295) OF 372 COMPOSED OF RX(35), RX(72), RX(109)  
RX(295) A + BU + DP ==> EX



EX  
YIELD 56%

RX(35) RCT A 181478-44-4, BU 87-62-7

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BV 774217-19-5

RX(72) RCT BV 774217-19-5

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

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RGT D 7732-18-5 Water  
CON cooled

PRO DL 774217-56-0  
NTE chemoselective

RX(109) RCT DL 774217-56-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

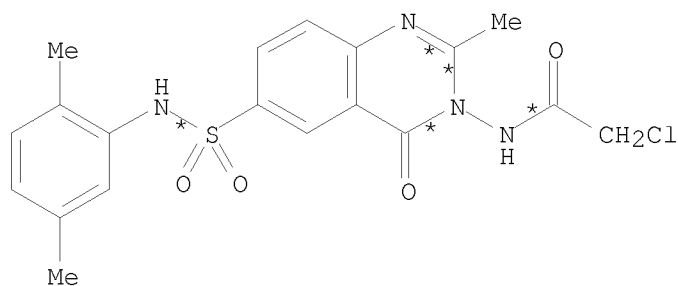
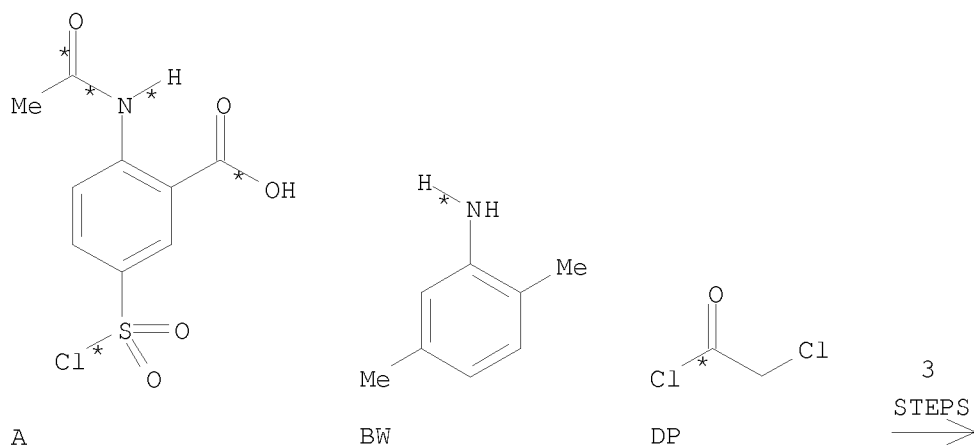
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EX 774217-94-6

RX(296) OF 372 COMPOSED OF RX(36), RX(73), RX(110)

RX(296) A + BW + DP ==> EY



EY  
YIELD 59%

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RX(36) RCT A 181478-44-4, BW 95-78-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BX 774217-20-8

RX(73) RCT BX 774217-20-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DM 774217-57-1

NTE chemoselective

RX(110) RCT DM 774217-57-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

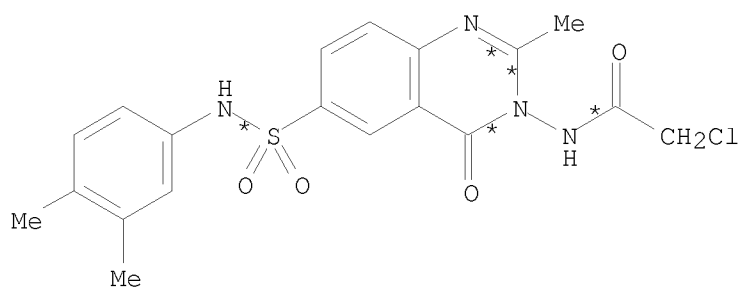
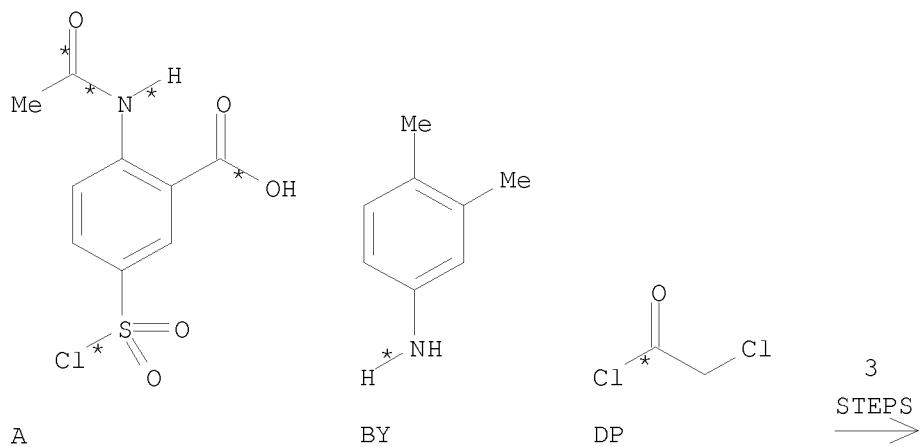
CON cooled

PRO EY 774217-95-7

RX(297) OF 372 COMPOSED OF RX(37), RX(74), RX(111)

RX(297) A + BY + DP ==> EZ

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EZ  
YIELD 62%

RX(37) RCT A 181478-44-4, BY 95-64-7

STAGE(1)  
CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO BZ 774217-21-9

RX(74) RCT BZ 774217-21-9

STAGE(1)  
RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water

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CON cooled

PRO DN 774217-58-2

NTE chemoselective

RX(111) RCT DN 774217-58-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

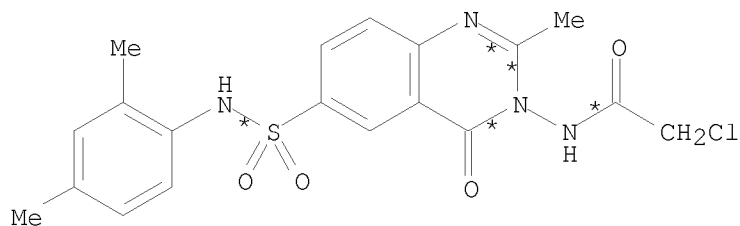
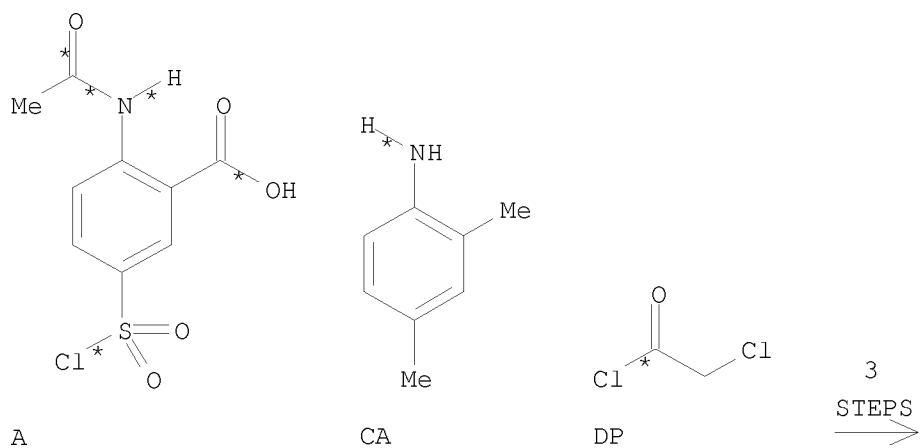
RGT D 7732-18-5 Water

CON cooled

PRO EZ 774217-96-8

RX(298) OF 372 COMPOSED OF RX(38), RX(75), RX(112)

RX(298) A + CA + DP ==> FA



FA  
YIELD 70%

RX(38) RCT A 181478-44-4, CA 95-68-1



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STAGE(1)  
CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CB 774217-22-0

RX(75) RCT CB 774217-22-0

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DO 774217-59-3  
NTE chemoselective

RX(112) RCT DO 774217-59-3, DP 79-04-9

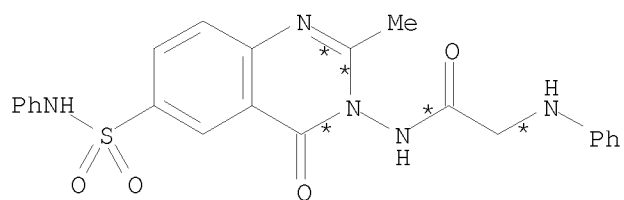
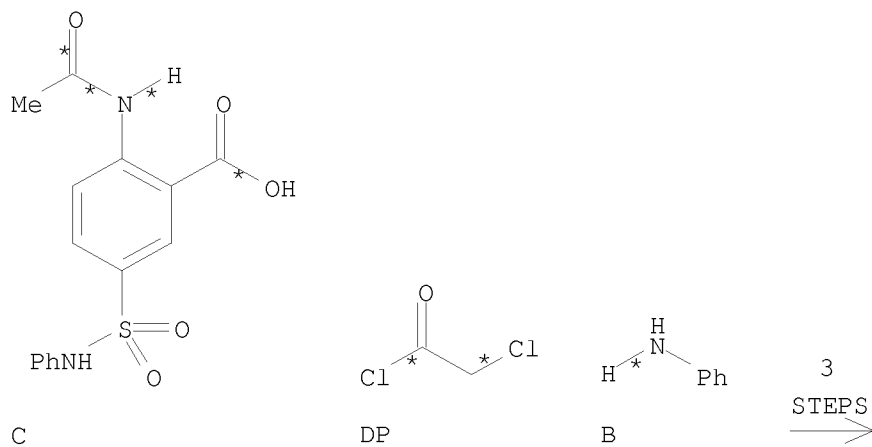
STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO FA 774217-97-9

RX(299) OF 372 COMPOSED OF RX(39), RX(76), RX(113)

RX(299) C + DP + B ==> FB



FB  
YIELD 52%

RX(39) RCT C 774216-86-3

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CC 774217-23-1  
NTE chemoselective

RX(76) RCT CC 774217-23-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

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PRO DQ 774217-60-6

RX(113) RCT B 62-53-3, DQ 774217-60-6

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

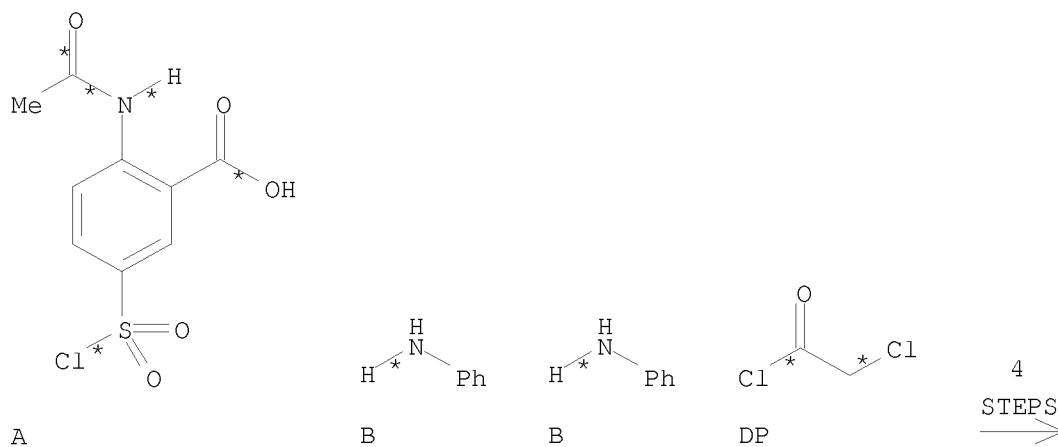
RGT D 7732-18-5 Water

CON cooled

PRO FB 774217-98-0

RX(300) OF 372 COMPOSED OF RX(1), RX(39), RX(76), RX(113)

RX(300) A + 2 B + DP ==> FB



FB  
YIELD 52%

RX(1) RCT A 181478-44-4, B 62-53-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO C 774216-86-3

RX(39) RCT C 774216-86-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CC 774217-23-1  
NTE chemoselective

RX(76) RCT CC 774217-23-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DQ 774217-60-6

RX(113) RCT B 62-53-3, DQ 774217-60-6

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

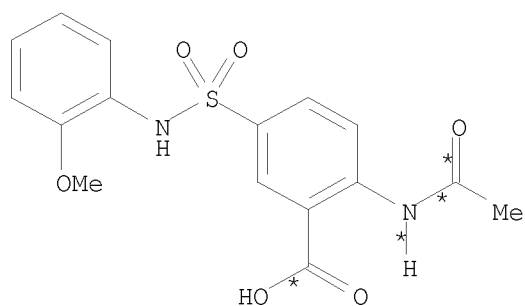
RGT D 7732-18-5 Water  
CON cooled

PRO FB 774217-98-0

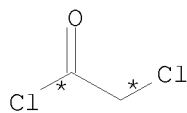
RX(301) OF 372 COMPOSED OF RX(40), RX(77), RX(114)

RX(301) H + DP + G ==> FC

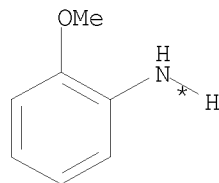
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H

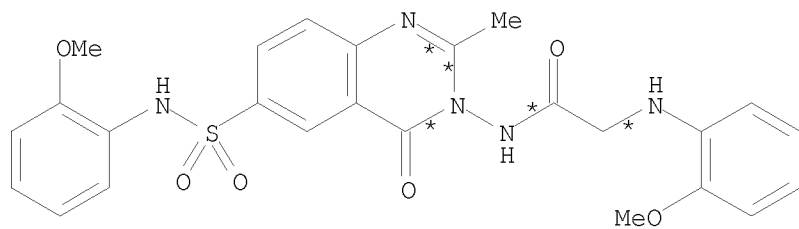


DP



G

3  
STEPS  
→



FC  
YIELD 51%

RX(40) RCT H 774216-87-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CF 774217-24-2

NTE chemoselective

RX(77) RCT CF 774217-24-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

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RGT D 7732-18-5 Water  
CON cooled

PRO DR 774217-61-7

RX(114) RCT G 90-04-0, DR 774217-61-7

STAGE (1)

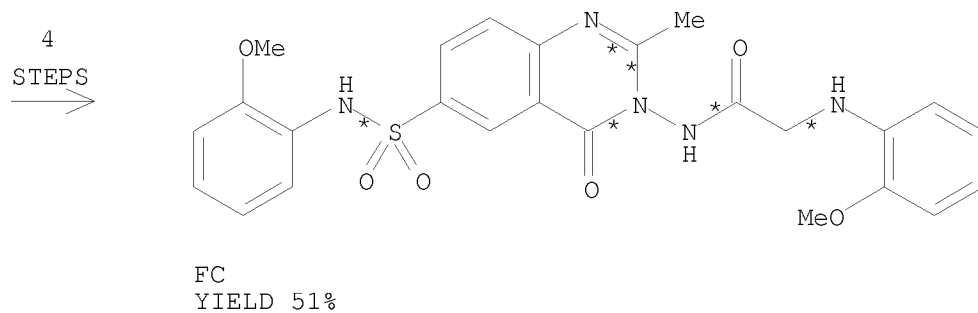
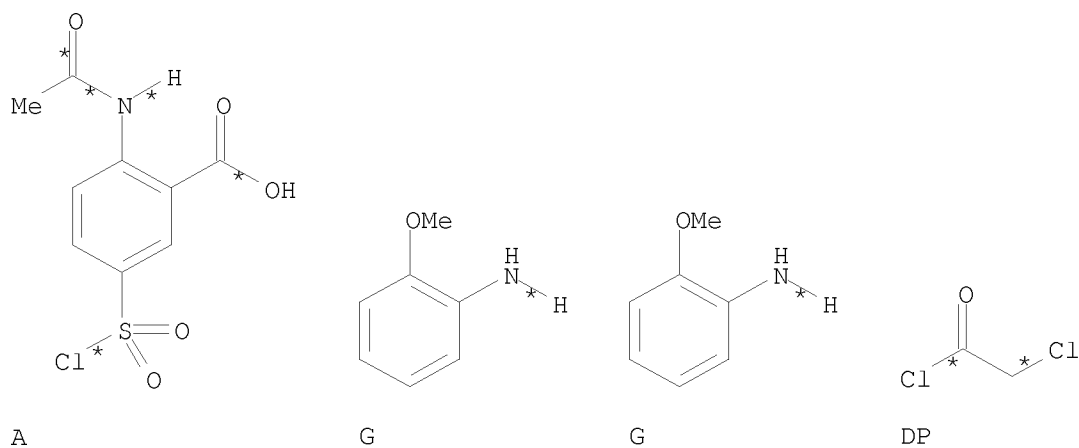
```
RGT  E 110-86-1 Pyridine
SOL  64-17-5 EtOH
CON  SUBSTAGE(1) 4 hours, 120 deg C
      SUBSTAGE(2) cooled
```

STAGE (2)

RGT D 7732-18-5 Water  
CON cooled

PRO FC 248259-39-4

RX(302) OF 372 COMPOSED OF RX(2), RX(40), RX(77), RX(114)

$$\text{RX}(302) \quad \text{A} + 2 \text{G} + \text{DP} \implies \text{FC}$$


RX(2) RCT A 181478-44-4, G 90-04-0

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STAGE(1)  
CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO H 774216-87-4

RX(40) RCT H 774216-87-4

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CF 774217-24-2  
NTE chemoselective

RX(77) RCT CF 774217-24-2, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DR 774217-61-7

RX(114) RCT G 90-04-0, DR 774217-61-7

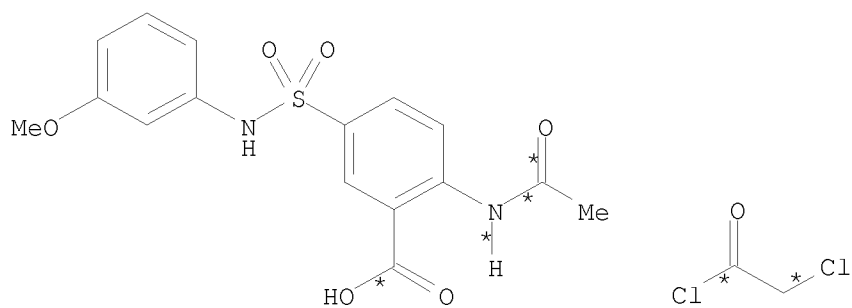
STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO FC 248259-39-4

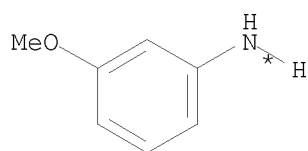
RX(303) OF 372 COMPOSED OF RX(41), RX(78), RX(115)  
RX(303) J + DP + I ==> FD

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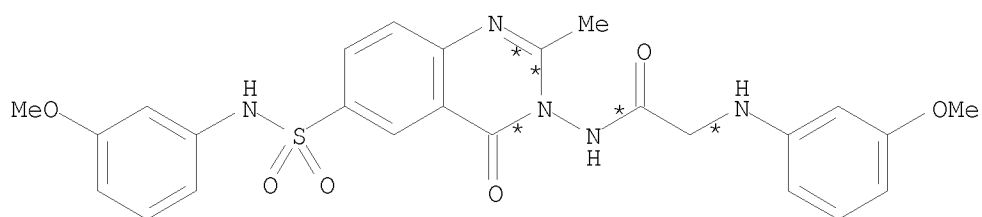
J

DP



I

3  
STEPS  
→



FD  
YIELD 54%

RX(41) RCT J 774216-88-5

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CG 774217-25-3

NTE chemoselective

RX(78) RCT CG 774217-25-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine



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SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DS 774217-62-8

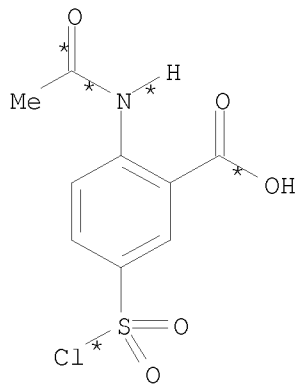
RX(115) RCT I 536-90-3, DS 774217-62-8

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

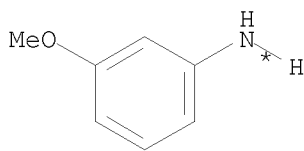
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO FD 774217-99-1

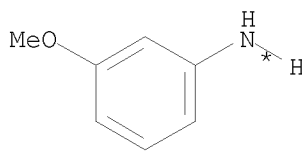
RX(304) OF 372 COMPOSED OF RX(3), RX(41), RX(78), RX(115)  
RX(304) A + 2 I + DP ==> FD



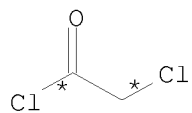
A



I



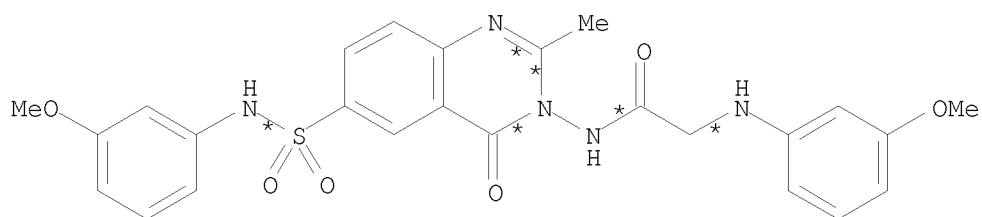
I



DP

4  
STEPS  
→

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FD  
YIELD 54%

RX(3) RCT A 181478-44-4, I 536-90-3

STAGE(1)

CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO J 774216-88-5

RX(41) RCT J 774216-88-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CG 774217-25-3  
NTE chemoselective

RX(78) RCT CG 774217-25-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DS 774217-62-8

RX(115) RCT I 536-90-3, DS 774217-62-8

STAGE(1)

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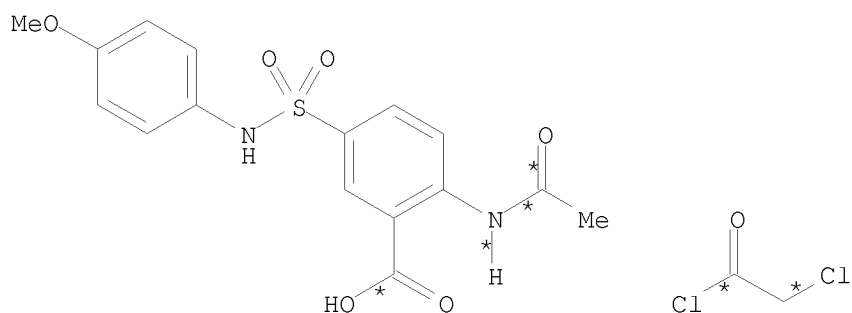
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

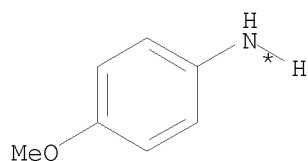
PRO FD 774217-99-1

RX(305) OF 372 COMPOSED OF RX(42), RX(79), RX(116)  
RX(305) L + DP + K ==> FE



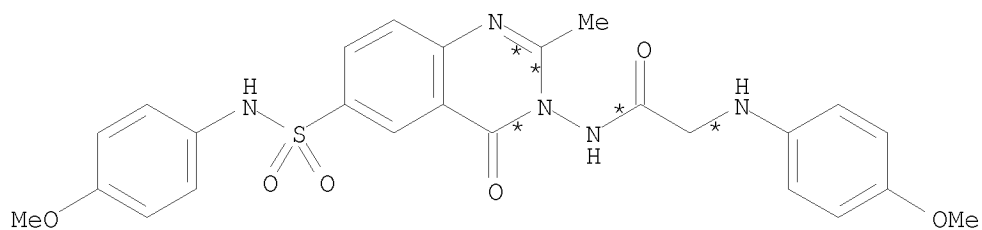
L

DP



K

3  
STEPS  
→



FE  
YIELD 51%

RX(42) RCT L 774216-89-6

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STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CH 774217-26-4  
NTE chemoselective

RX(79) RCT CH 774217-26-4, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DT 774217-63-9

RX(116) RCT K 104-94-9, DT 774217-63-9

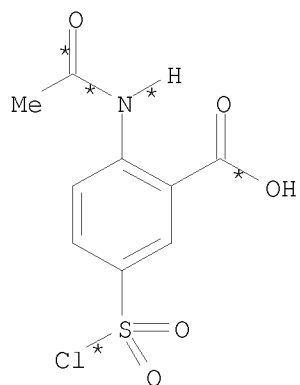
STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

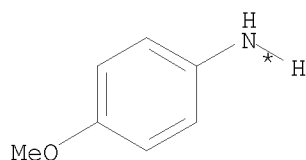
PRO FE 248259-41-8

RX(306) OF 372 COMPOSED OF RX(4), RX(42), RX(79), RX(116)

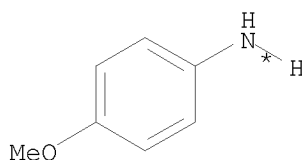
RX(306) A + 2 K + DP ==> FE



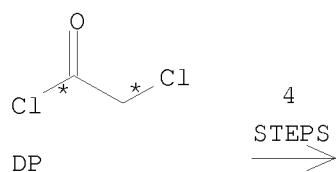
A



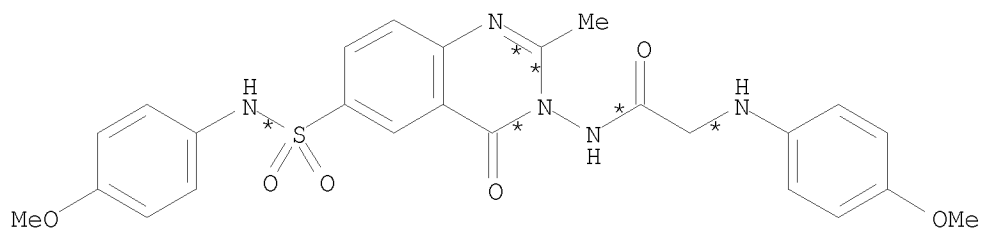
K



K



DP



FE  
YIELD 51%

RX(4) RCT A 181478-44-4, K 104-94-9

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO L 774216-89-6

RX(42) RCT L 774216-89-6

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STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CH 774217-26-4  
NTE chemoselective

RX(79) RCT CH 774217-26-4, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DT 774217-63-9

RX(116) RCT K 104-94-9, DT 774217-63-9

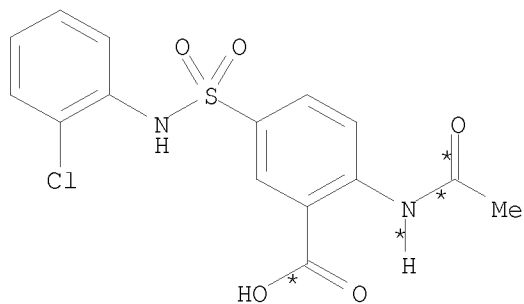
STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

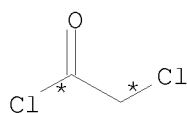
PRO FE 248259-41-8

RX(307) OF 372 COMPOSED OF RX(43), RX(80), RX(117)

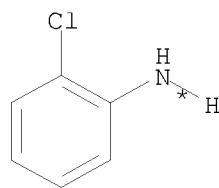
RX(307) N + DP + M ==> FF



N



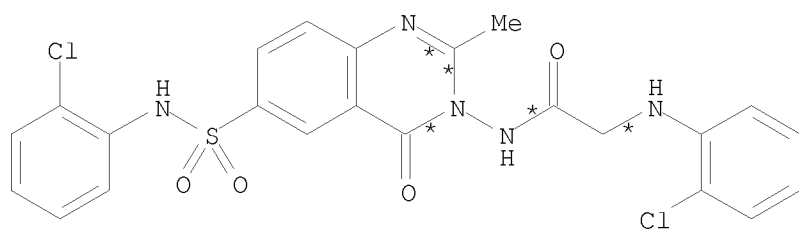
DP



M

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3  
STEPS  
→



FF  
YIELD 58%

RX(43) RCT N 774216-90-9

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CI 774217-27-5  
NTE chemoselective

RX(80) RCT CI 774217-27-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DU 774217-64-0

RX(117) RCT M 95-51-2, DU 774217-64-0

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

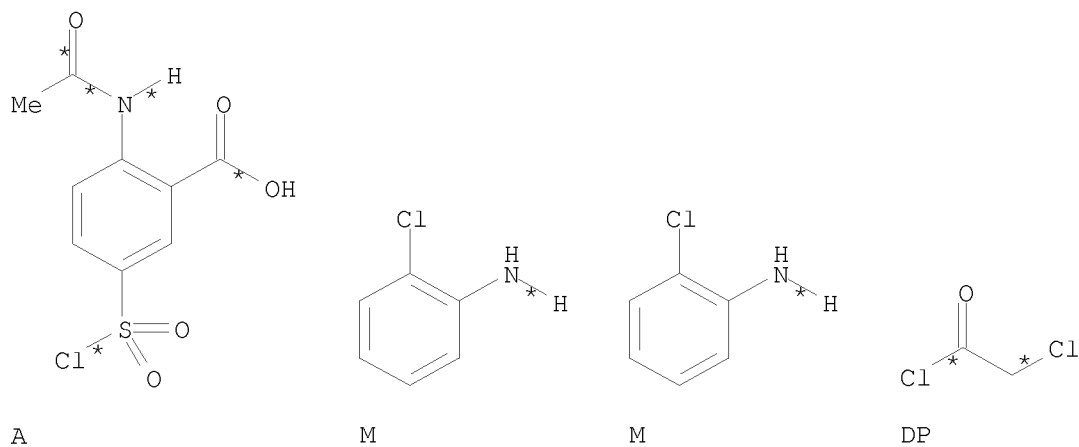
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

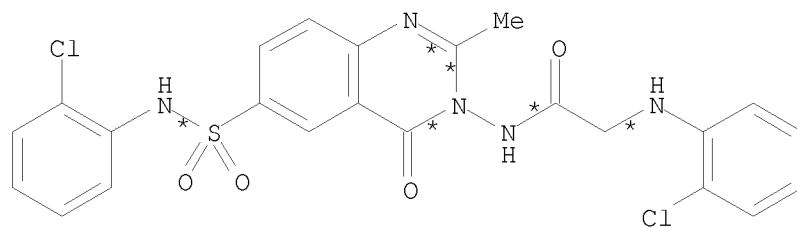
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PRO FF 248259-42-9

RX(308) OF 372 COMPOSED OF RX(5), RX(43), RX(80), RX(117)  
RX(308) A + 2 M + DP ==> FF



4  
STEPS  
→



FF  
YIELD 58%

RX(5) RCT A 181478-44-4, M 95-51-2

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO N 774216-90-9

RX(43) RCT N 774216-90-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O



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SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CI 774217-27-5  
NTE chemoselective

RX(80) RCT CI 774217-27-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DU 774217-64-0

RX(117) RCT M 95-51-2, DU 774217-64-0

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

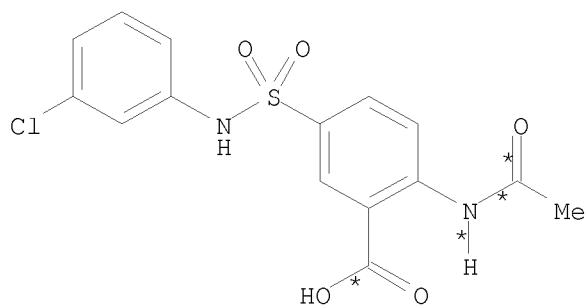
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

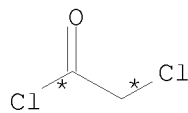
PRO FF 248259-42-9

RX(309) OF 372 COMPOSED OF RX(44), RX(81), RX(118)

RX(309) P + DP + O ==> FG

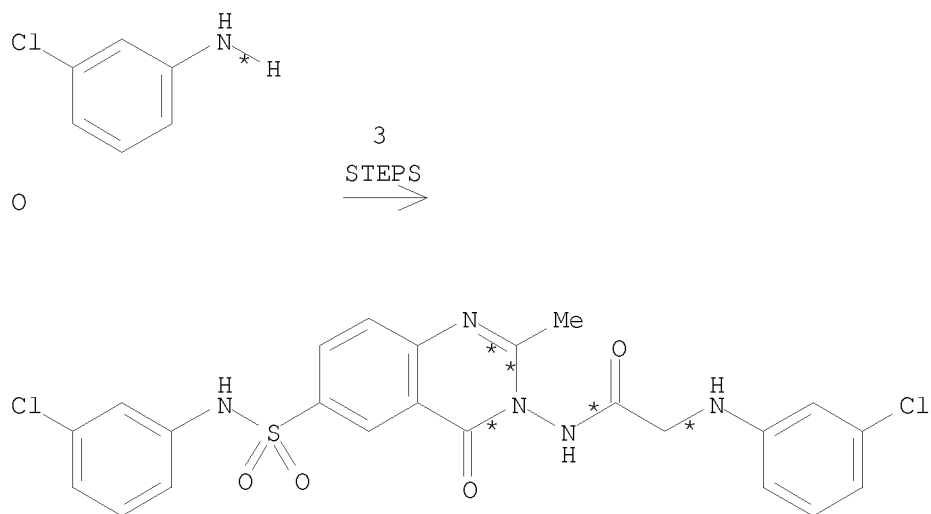


P



DP

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FG  
YIELD 58%

RX(44) RCT P 774216-91-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CJ 774217-28-6  
NTE chemoselective

RX(81) RCT CJ 774217-28-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DV 774217-65-1

RX(118) RCT O 108-42-9, DV 774217-65-1

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

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STAGE(2)

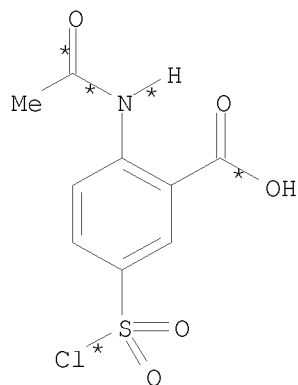
RGT D 7732-18-5 Water

CON cooled

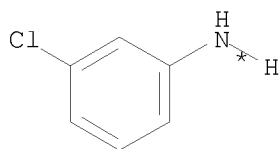
PRO FG 774218-00-7

RX(310) OF 372 COMPOSED OF RX(6), RX(44), RX(81), RX(118)

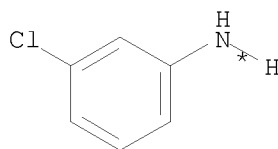
RX(310) A + 2 O + DP ==> FG



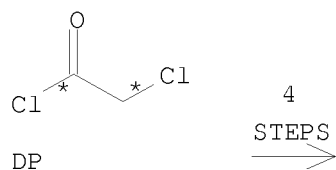
A



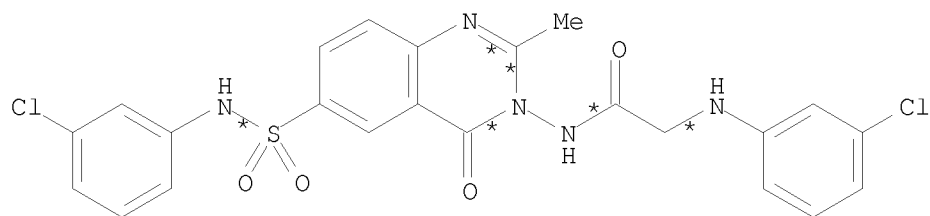
O



O



4  
STEPS  
→



FG  
YIELD 58%

RX(6) RCT A 181478-44-4, O 108-42-9

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

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SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO P 774216-91-0

RX(44) RCT P 774216-91-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CJ 774217-28-6  
NTE chemoselective

RX(81) RCT CJ 774217-28-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DV 774217-65-1

RX(118) RCT O 108-42-9, DV 774217-65-1

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

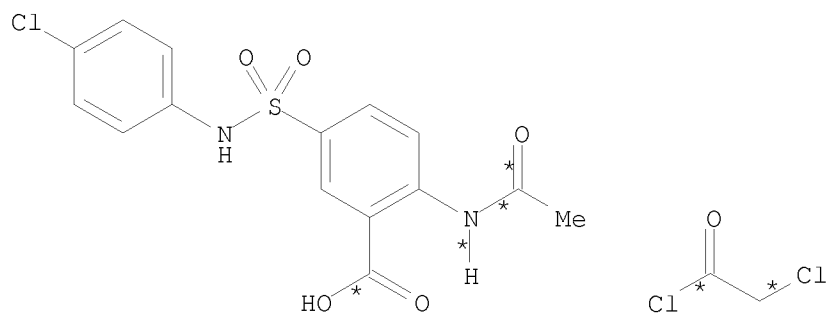
RGT D 7732-18-5 Water  
CON cooled

PRO FG 774218-00-7

RX(311) OF 372 COMPOSED OF RX(45), RX(82), RX(119)

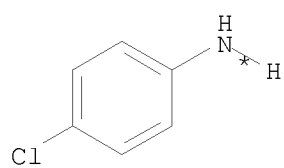
RX(311) R + DP + Q ==> FH

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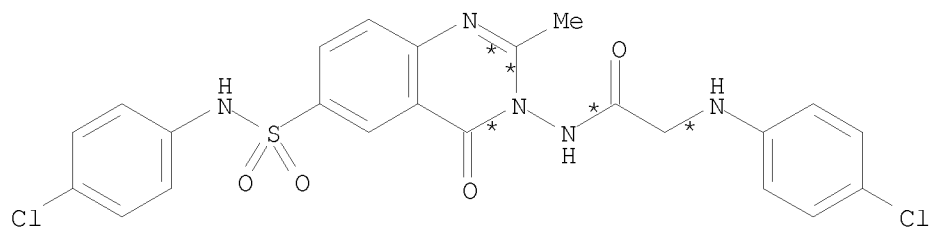
R

DP



Q

3  
STEPS  
→



FH  
YIELD 62%

RX(45) RCT R 774216-92-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CK 774217-29-7  
NTE chemoselective

RX(82) RCT CK 774217-29-7, DP 79-04-9

STAGE(1)

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RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DW 774217-66-2

RX(119) RCT Q 106-47-8, DW 774217-66-2

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

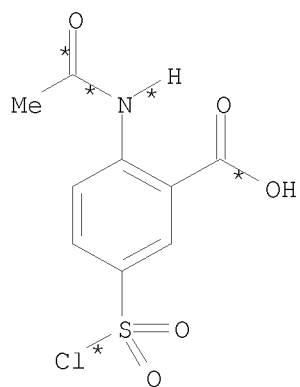
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

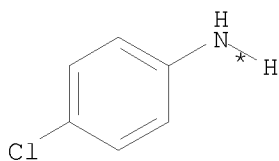
PRO FH 248259-43-0

RX(312) OF 372 COMPOSED OF RX(7), RX(45), RX(82), RX(119)

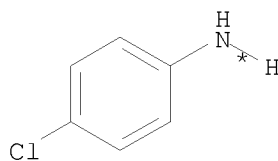
RX(312) A + 2 Q + DP ==> FH



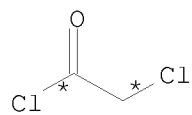
A



Q



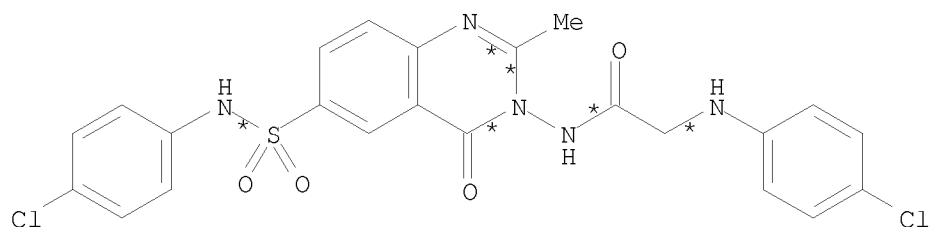
Q



DP

4  
STEPS  
→

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FH  
YIELD 62%

RX(7) RCT A 181478-44-4, Q 106-47-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO R 774216-92-1

RX(45) RCT R 774216-92-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CK 774217-29-7

NTE chemoselective

RX(82) RCT CK 774217-29-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DW 774217-66-2

RX(119) RCT Q 106-47-8, DW 774217-66-2

STAGE(1)

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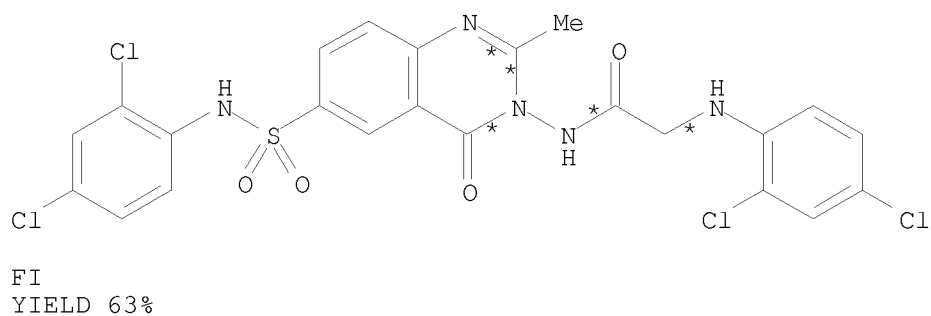
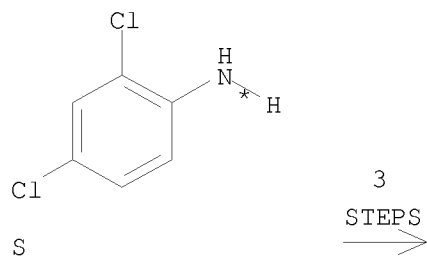
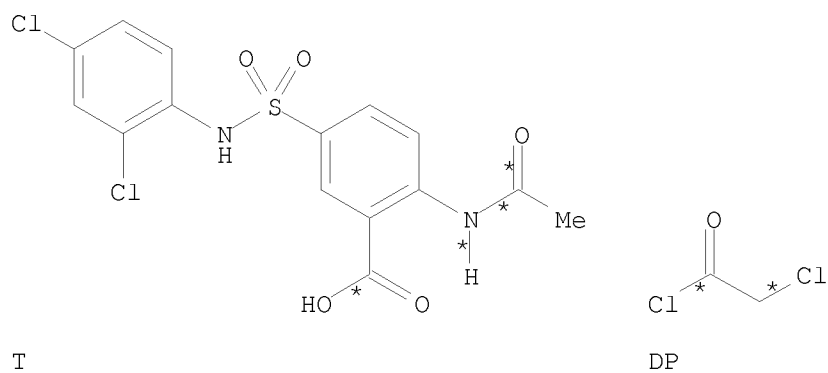
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO FH 248259-43-0

RX(313) OF 372 COMPOSED OF RX(46), RX(83), RX(120)  
RX(313) T + DP + S ==> FI





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RX(46) RCT T 774216-93-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CL 774217-30-0  
NTE chemoselective

RX(83) RCT CL 774217-30-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DX 774217-67-3

RX(120) RCT S 554-00-7, DX 774217-67-3

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

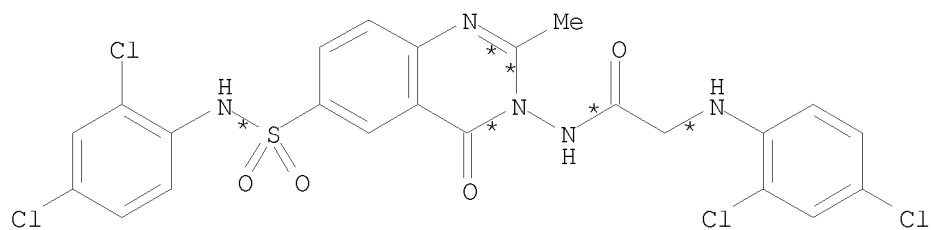
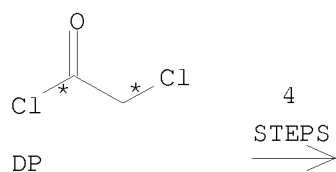
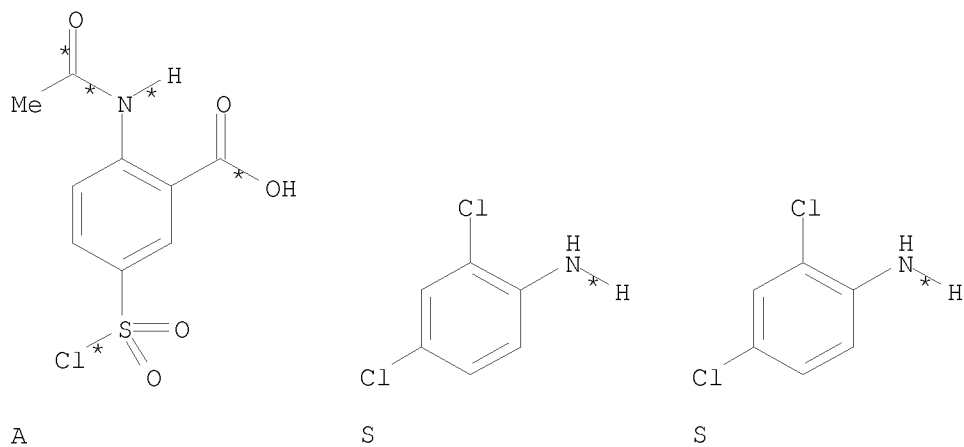
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO FI 774218-01-8

RX(314) OF 372 COMPOSED OF RX(8), RX(46), RX(83), RX(120)  
RX(314) A + 2 S + DP ==> FI

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FI  
YIELD 63%

RX(8) RCT A 181478-44-4, S 554-00-7

STAGE(1)

CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO T 774216-93-2

RX(46) RCT T 774216-93-2

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STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CL 774217-30-0  
NTE chemoselective

RX(83) RCT CL 774217-30-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DX 774217-67-3

RX(120) RCT S 554-00-7, DX 774217-67-3

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

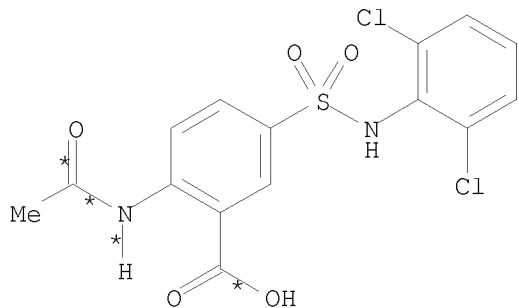
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

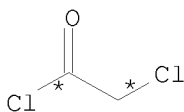
PRO FI 774218-01-8

RX(315) OF 372 COMPOSED OF RX(47), RX(84), RX(121)

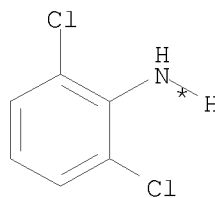
RX(315) V + DP + U ==> FJ



V



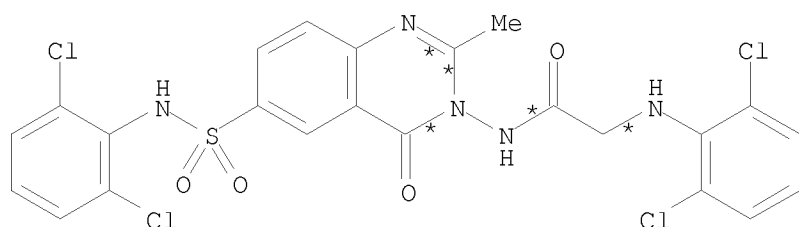
DP



U

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3  
STEPS  
→



FJ  
YIELD 61%

RX(47) RCT V 774216-94-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CM 774217-31-1  
NTE chemoselective

RX(84) RCT CM 774217-31-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DY 774217-68-4

RX(121) RCT U 608-31-1, DY 774217-68-4

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

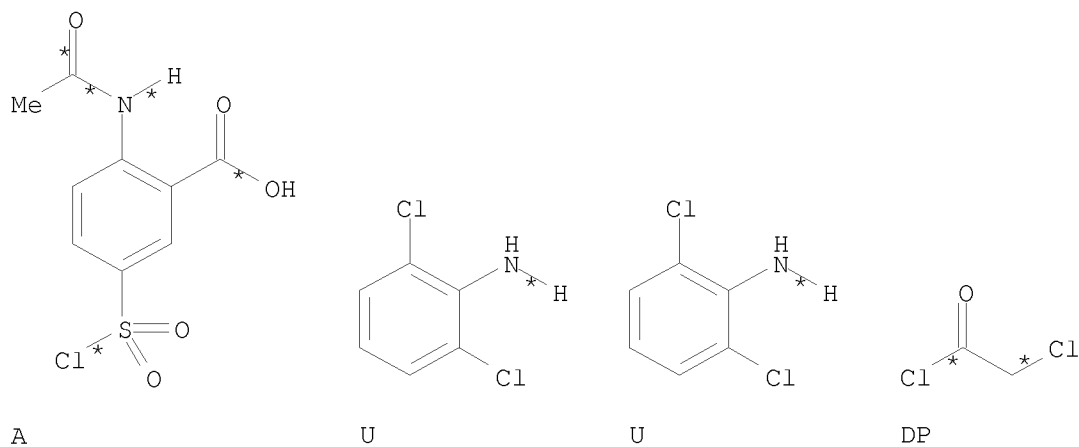
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

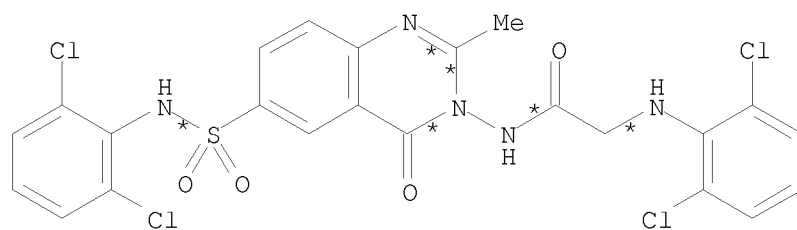
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PRO FJ 774218-02-9

RX(316) OF 372 COMPOSED OF RX(9), RX(47), RX(84), RX(121)  
RX(316) A + 2 U + DP ==> FJ



4  
STEPS  
→



FJ  
YIELD 61%

RX(9) RCT A 181478-44-4, U 608-31-1

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO V 774216-94-3

RX(47) RCT V 774216-94-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

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SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CM 774217-31-1  
NTE chemoselective

RX(84) RCT CM 774217-31-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DY 774217-68-4

RX(121) RCT U 608-31-1, DY 774217-68-4

STAGE(1)

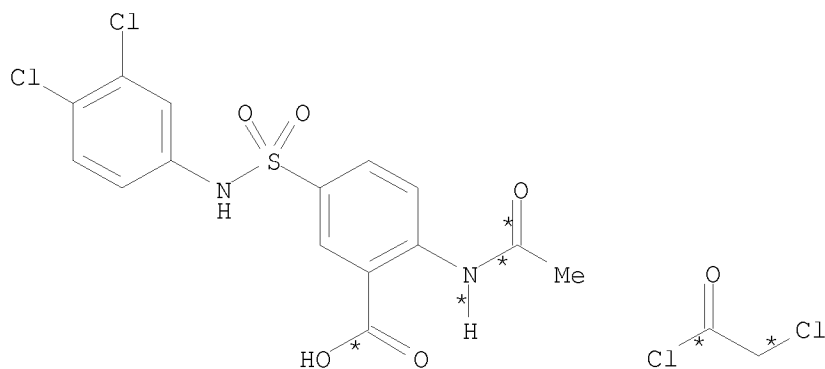
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO FJ 774218-02-9

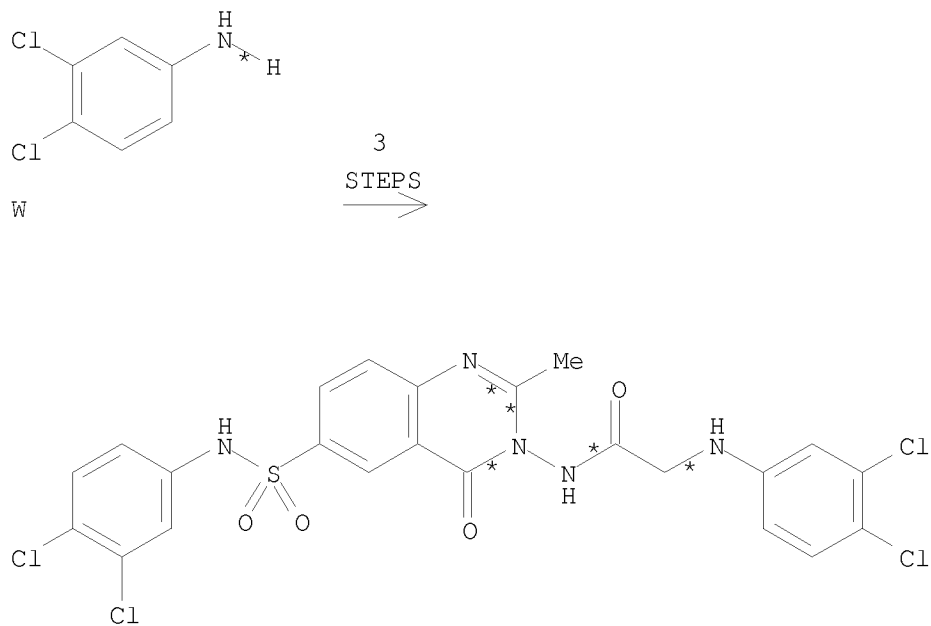
RX(317) OF 372 COMPOSED OF RX(48), RX(85), RX(122)  
RX(317) X + DP + W ==> FK



X

DP

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FK  
YIELD 64%

RX(48) RCT X 774216-95-4

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CN 774217-32-2  
NTE chemoselective

RX(85) RCT CN 774217-32-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DZ 774217-69-5

RX(122) RCT W 95-76-1, DZ 774217-69-5

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STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

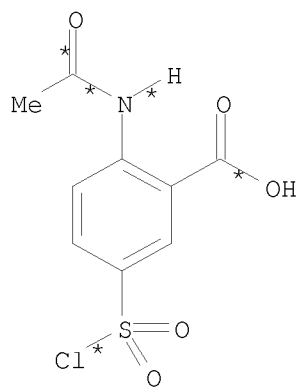
RGT D 7732-18-5 Water

CON cooled

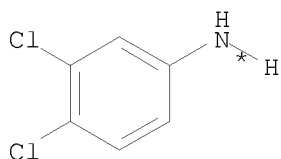
PRO FK 774218-03-0

RX(318) OF 372 COMPOSED OF RX(10), RX(48), RX(85), RX(122)

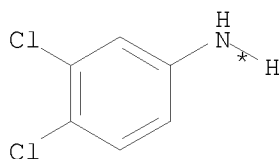
RX(318) A + 2 W + DP ==> FK



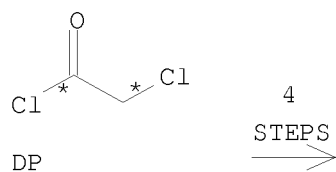
A



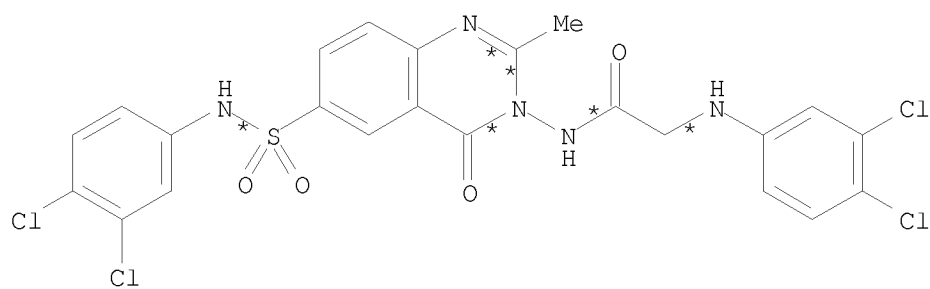
W



W



DP



FK

YIELD 64%



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RX(10) RCT A 181478-44-4, W 95-76-1

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO X 774216-95-4

RX(48) RCT X 774216-95-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CN 774217-32-2

NTE chemoselective

RX(85) RCT CN 774217-32-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DZ 774217-69-5

RX(122) RCT W 95-76-1, DZ 774217-69-5

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

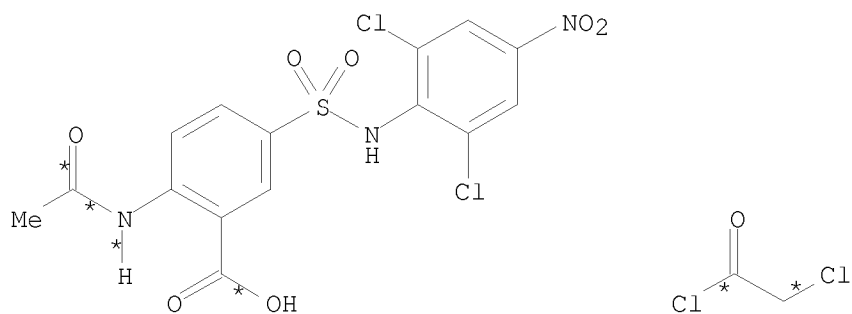
CON cooled

PRO FK 774218-03-0

RX(319) OF 372 COMPOSED OF RX(49), RX(86), RX(123)

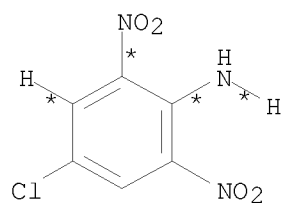
10/ 562,112

RX(319)    Z    +    DP    +    Y    ==>    FL



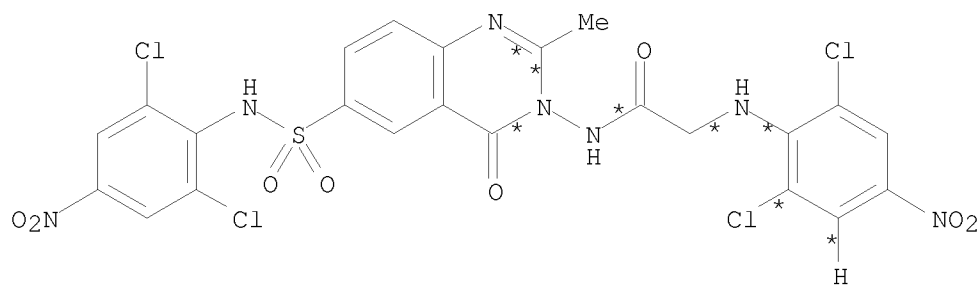
Z

DP



Y

3  
STEPS  
=>



FL  
YIELD 67%

RX(49)    RCT    Z 218617-81-3

STAGE(1)

RGT    CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL    67-56-1 MeOH  
CON    3 hours, reflux

STAGE(2)

RGT    D 7732-18-5 Water  
CON    cooled

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PRO CO 234096-58-3  
NTE chemoselective

RX(86) RCT CO 234096-58-3, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EA 774217-70-8

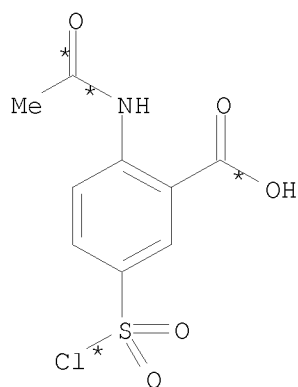
RX(123) RCT Y 5388-62-5, EA 774217-70-8

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

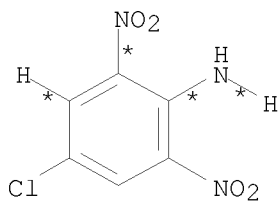
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO FL 774218-04-1

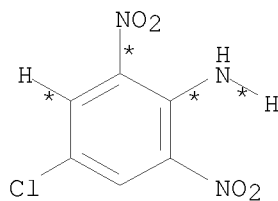
RX(320) OF 372 COMPOSED OF RX(11), RX(49), RX(86), RX(123)  
RX(320) A + 2 Y + DP ==> FL



A

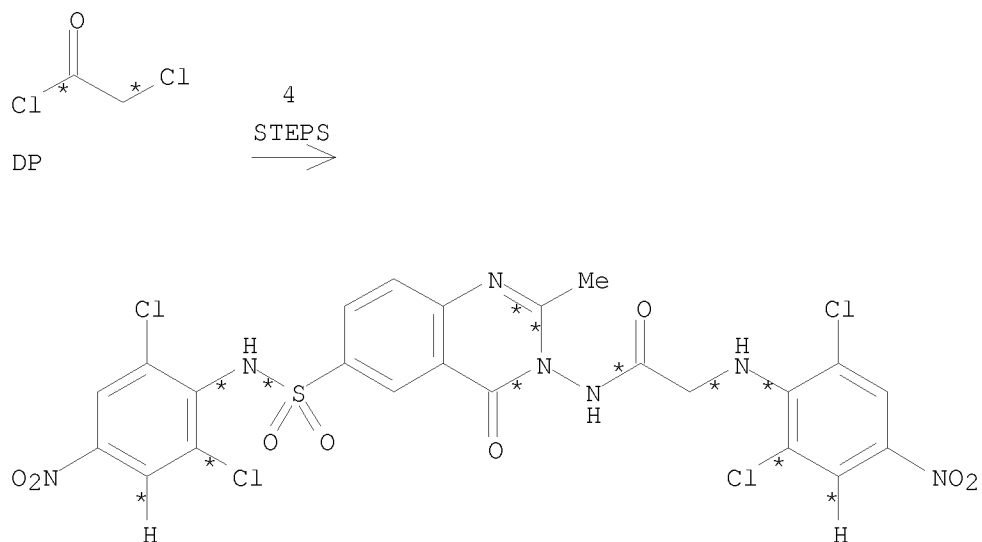


Y



Y

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FL  
YIELD 67%

RX(11) RCT A 181478-44-4, Y 5388-62-5

STAGE(1)

CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO Z 218617-81-3

RX(49) RCT Z 218617-81-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CO 234096-58-3  
NTE chemoselective

RX(86) RCT CO 234096-58-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C

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SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EA 774217-70-8

RX(123) RCT Y 5388-62-5, EA 774217-70-8

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

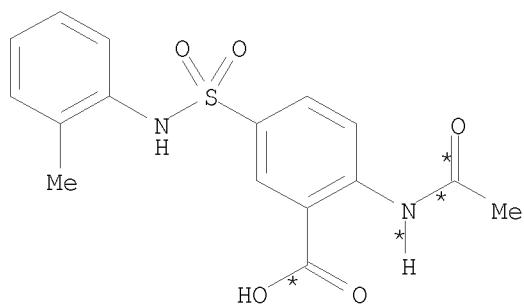
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

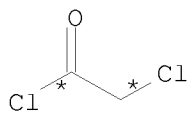
PRO FL 774218-04-1

RX(321) OF 372 COMPOSED OF RX(50), RX(87), RX(124)

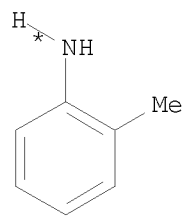
RX(321) AB + DP + AA ==> FM



AB



DP

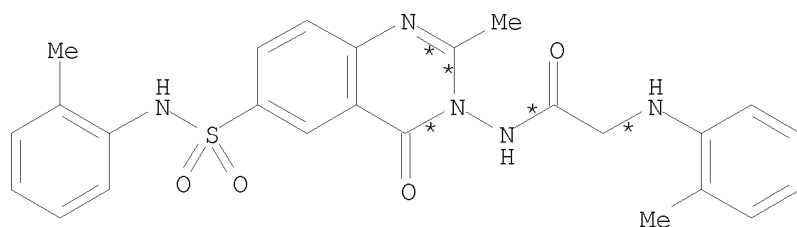


AA

3

STEPS  
→

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FM  
YIELD 54%

RX(50) RCT AB 774216-96-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CP 774217-33-3  
NTE chemoselective

RX(87) RCT CP 774217-33-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EB 774217-71-9

RX(124) RCT AA 95-53-4, EB 774217-71-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

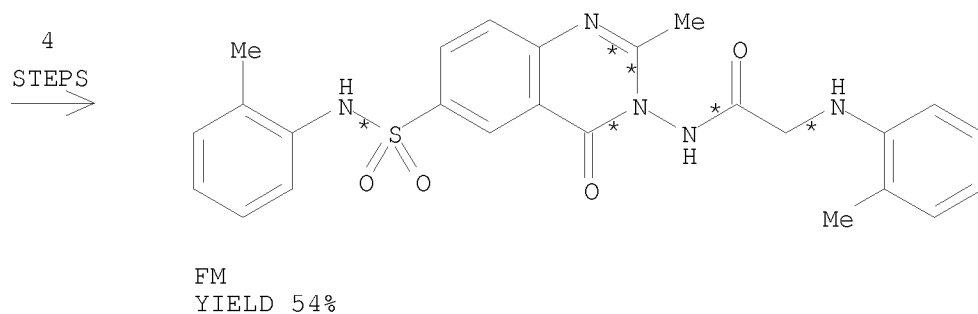
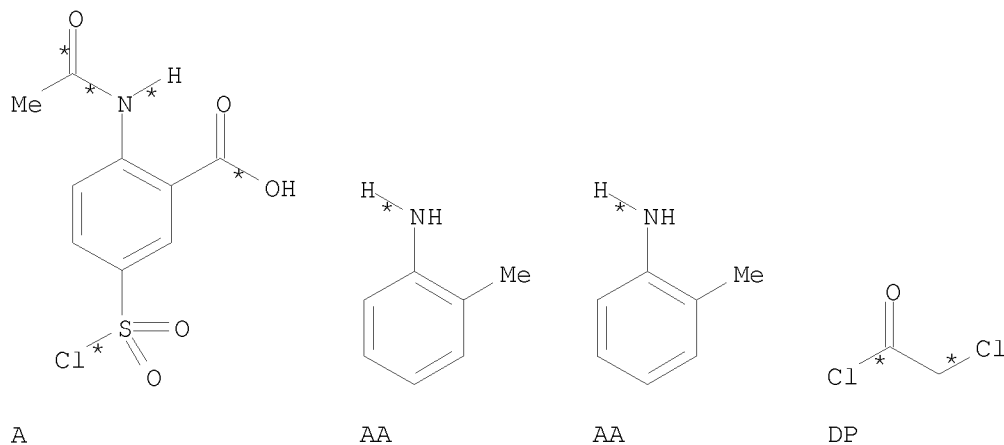
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO FM 774218-05-2

RX(322) OF 372 COMPOSED OF RX(12), RX(50), RX(87), RX(124)  
RX(322) A + 2 AA + DP ==> FM

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RX(12) RCT A 181478-44-4, AA 95-53-4

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AB 774216-96-5

RX(50) RCT AB 774216-96-5

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CP 774217-33-3  
NTE chemoselective

RX(87) RCT CP 774217-33-3, DP 79-04-9

```

STAGE(1)
  RGT  E 110-86-1 Pyridine
  SOL  64-17-5 EtOH
  CON  SUBSTAGE(1) 4 hours, 120 deg C
      SUBSTAGE(2) cooled

```

```
STAGE(2)
      RGT  D 7732-18-5 Water
      CON  cooled
```

PRO EB 774217-71-9

RX(124) RCT AA 95-53-4, EB 774217-71-9

```

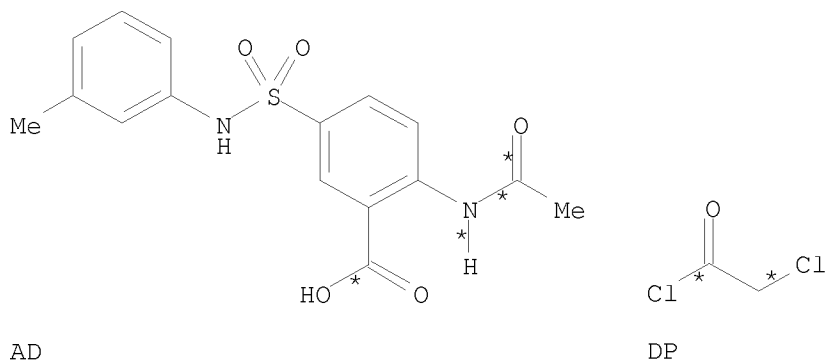
STAGE(1)
  RGT  E 110-86-1 Pyridine
  SOL  64-17-5 EtOH
  CON  SUBSTAGE(1) 4 hours, 120 deg C
      SUBSTAGE(2) cooled

```

STAGE (2)  
RGT D 7732-18-5 Water  
CON cooled

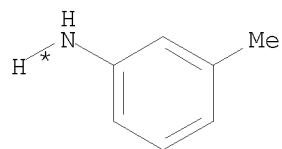
PRO FM 774218-05-2

RX(323) OF 372 COMPOSED OF RX(51), RX(88), RX(125)  
RX(323) AD + DP + AC ==> FN



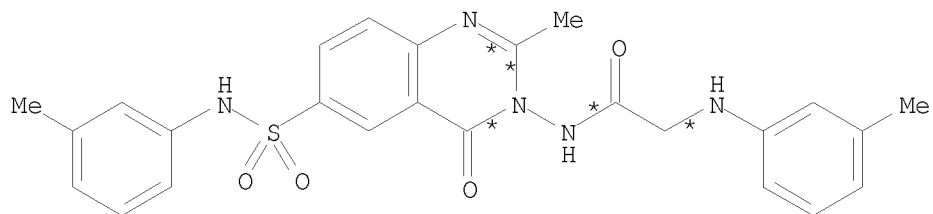


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AC

3  
STEPS  
→



FN  
YIELD 55%

RX(51) RCT AD 774216-97-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CQ 774217-34-4  
NTE chemoselective

RX(88) RCT CQ 774217-34-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EC 774217-72-0

RX(125) RCT AC 108-44-1, EC 774217-72-0

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

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STAGE(2)

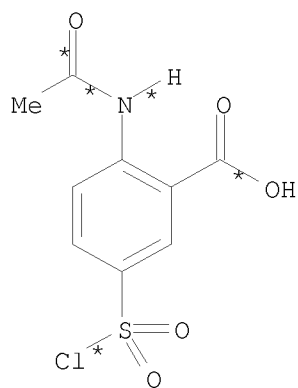
RGT D 7732-18-5 Water

CON cooled

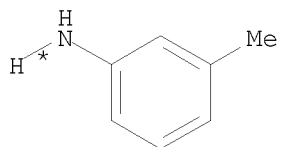
PRO FN 774218-06-3

RX(324) OF 372 COMPOSED OF RX(13), RX(51), RX(88), RX(125)

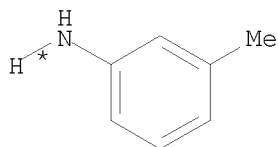
RX(324) A + 2 AC + DP ==> FN



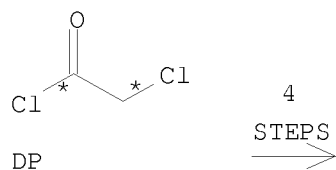
A



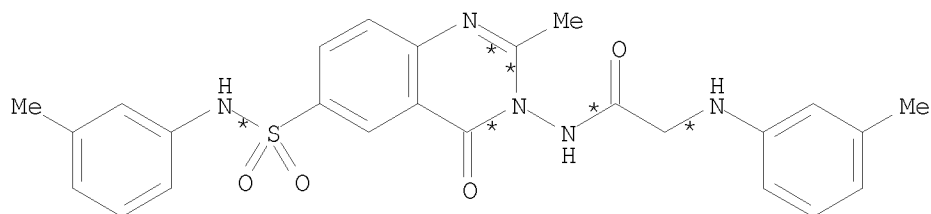
AC



AC



DP



FN

YIELD 55%

RX(13) RCT A 181478-44-4, AC 108-44-1

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

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CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO AD 774216-97-6

RX(51) RCT AD 774216-97-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CQ 774217-34-4  
NTE chemoselective

RX(88) RCT CQ 774217-34-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EC 774217-72-0

RX(125) RCT AC 108-44-1, EC 774217-72-0

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

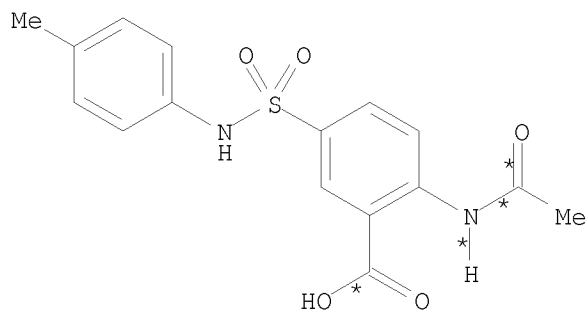
RGT D 7732-18-5 Water  
CON cooled

PRO FN 774218-06-3

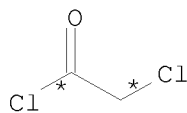
RX(325) OF 372 COMPOSED OF RX(52), RX(89), RX(126)

RX(325) AF + DP + AE ==> FO

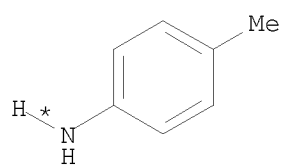
10/ 562,112



AF

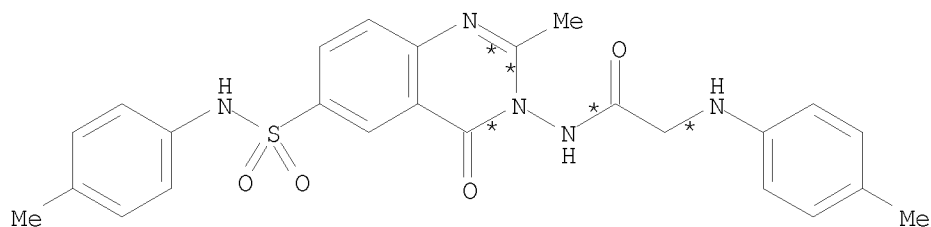


DP



AE

3  
STEPS  
→



FO  
YIELD 52%

RX(52) RCT AF 774216-98-7

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CR 774217-35-5  
NTE chemoselective

RX(89) RCT CR 774217-35-5, DP 79-04-9

STAGE(1)

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RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO ED 774217-73-1

RX(126) RCT AE 106-49-0, ED 774217-73-1

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

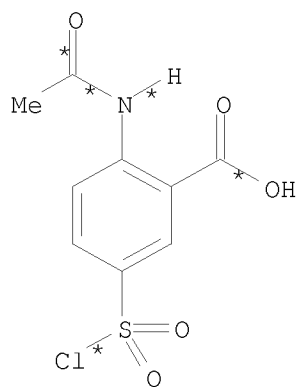
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

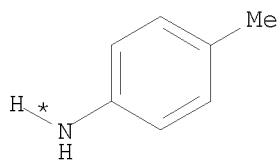
PRO FO 774218-07-4

RX(326) OF 372 COMPOSED OF RX(14), RX(52), RX(89), RX(126)

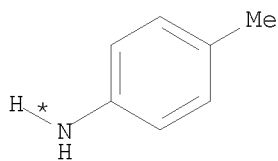
RX(326) A + 2 AE + DP ==> FO



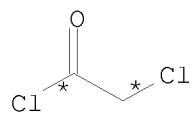
A



AE



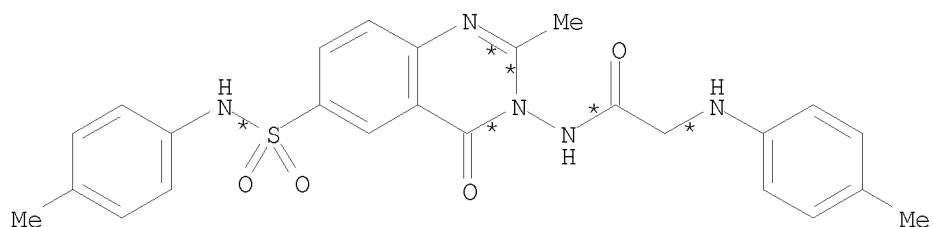
AE



DP

4  
STEPS  
→

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FO  
YIELD 52%

RX(14) RCT A 181478-44-4, AE 106-49-0

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AF 774216-98-7

RX(52) RCT AF 774216-98-7

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CR 774217-35-5

NTE chemoselective

RX(89) RCT CR 774217-35-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO ED 774217-73-1

RX(126) RCT AE 106-49-0, ED 774217-73-1

STAGE(1)

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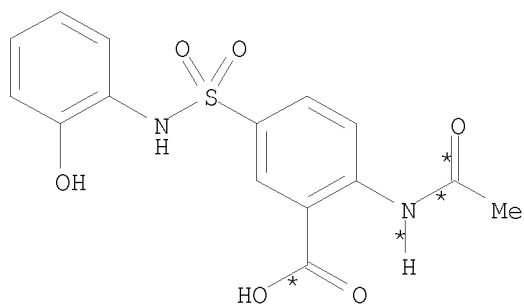
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

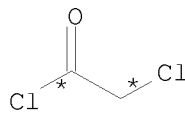
RGT D 7732-18-5 Water  
CON cooled

PRO FO 774218-07-4

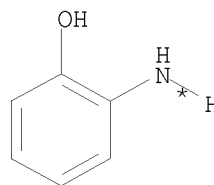
RX(327) OF 372 COMPOSED OF RX(53), RX(90), RX(127)  
RX(327) AH + DP + AG ==> FP



AH

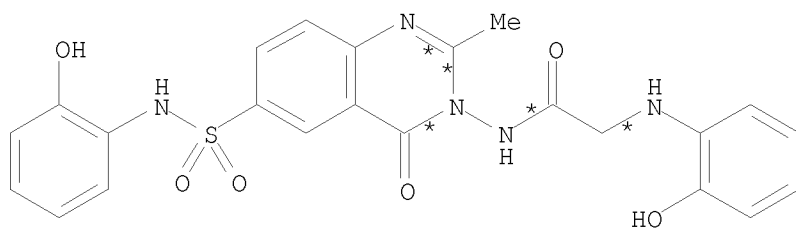


DP



AG

3  
STEPS  
=>



FP  
YIELD 56%

RX(53) RCT AH 774216-99-8

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

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RGT D 7732-18-5 Water  
CON cooled

PRO CS 774217-36-6  
NTE chemoselective

RX(90) RCT CS 774217-36-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EE 774217-74-2

RX(127) RCT AG 95-55-6, EE 774217-74-2

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

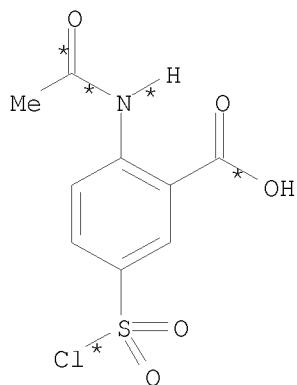
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

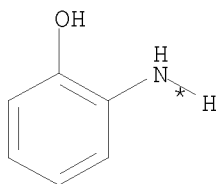
PRO FP 774218-08-5

RX(328) OF 372 COMPOSED OF RX(15), RX(53), RX(90), RX(127)

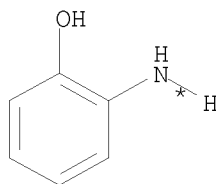
RX(328) A + 2 AG + DP ==> FP



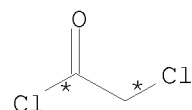
A



AG



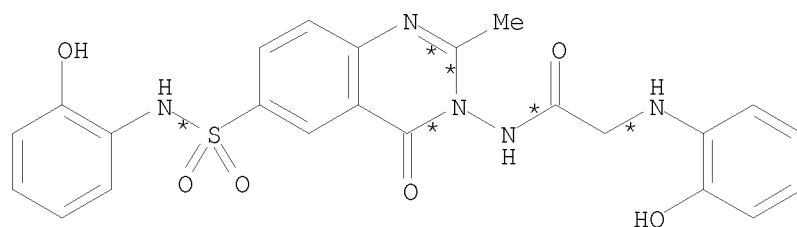
AG



DP



4  
STEPS  
→



FP  
YIELD 56%

RX(15) RCT A 181478-44-4, AG 95-55-6

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AH 774216-99-8

RX(53) RCT AH 774216-99-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CS 774217-36-6

NTE chemoselective

RX(90) RCT CS 774217-36-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EE 774217-74-2

RX(127) RCT AG 95-55-6, EE 774217-74-2

STAGE(1)

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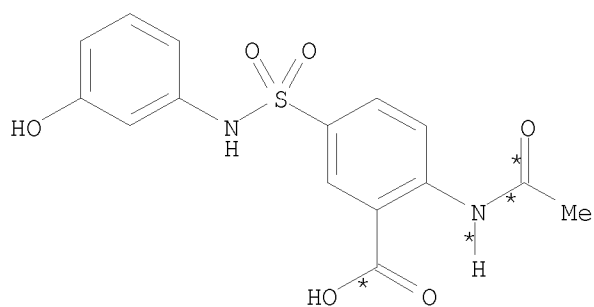
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

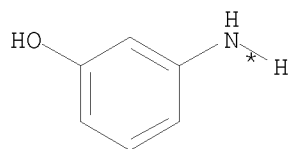
PRO FP 774218-08-5

RX(329) OF 372 COMPOSED OF RX(54), RX(91), RX(128)  
RX(329) AJ + DP + AI ==> FQ



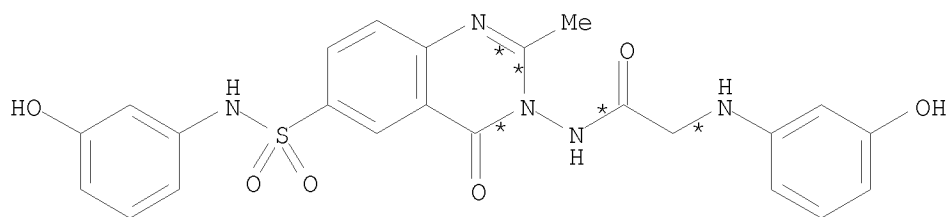
AJ

DP



AI

3  
STEPS  
→



FQ  
YIELD 57%

RX(54) RCT AJ 774217-00-4

STAGE(1)

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RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CT 774217-37-7  
NTE chemoselective

RX(91) RCT CT 774217-37-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EF 774217-75-3

RX(128) RCT AI 591-27-5, EF 774217-75-3

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

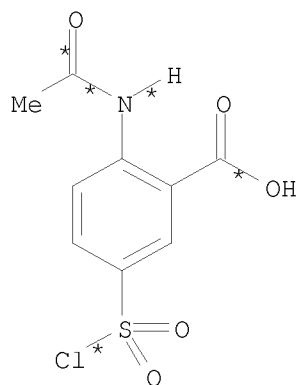
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

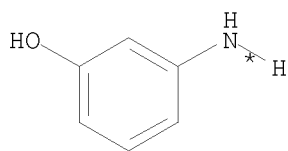
PRO FQ 774218-09-6

RX(330) OF 372 COMPOSED OF RX(16), RX(54), RX(91), RX(128)

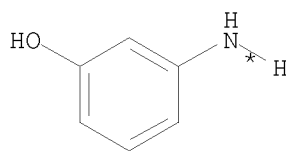
RX(330) A + 2 AI + DP ==> FQ



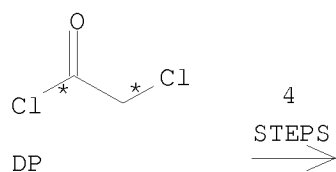
A



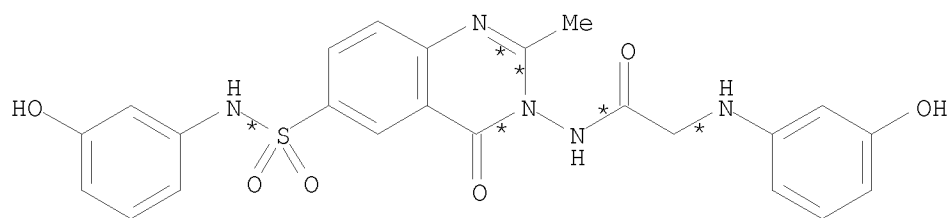
AI



AI



DP



FQ

YIELD 57%

RX(16) RCT A 181478-44-4, AI 591-27-5

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AJ 774217-00-4

RX(54) RCT AJ 774217-00-4

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STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CT 774217-37-7  
NTE chemoselective

RX(91) RCT CT 774217-37-7, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EF 774217-75-3

RX(128) RCT AI 591-27-5, EF 774217-75-3

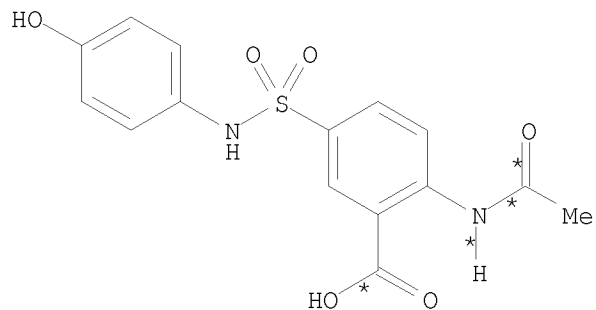
STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

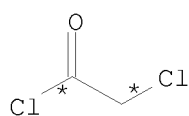
PRO FQ 774218-09-6

RX(331) OF 372 COMPOSED OF RX(55), RX(92), RX(129)

RX(331) AL + DP + AK ==> FR

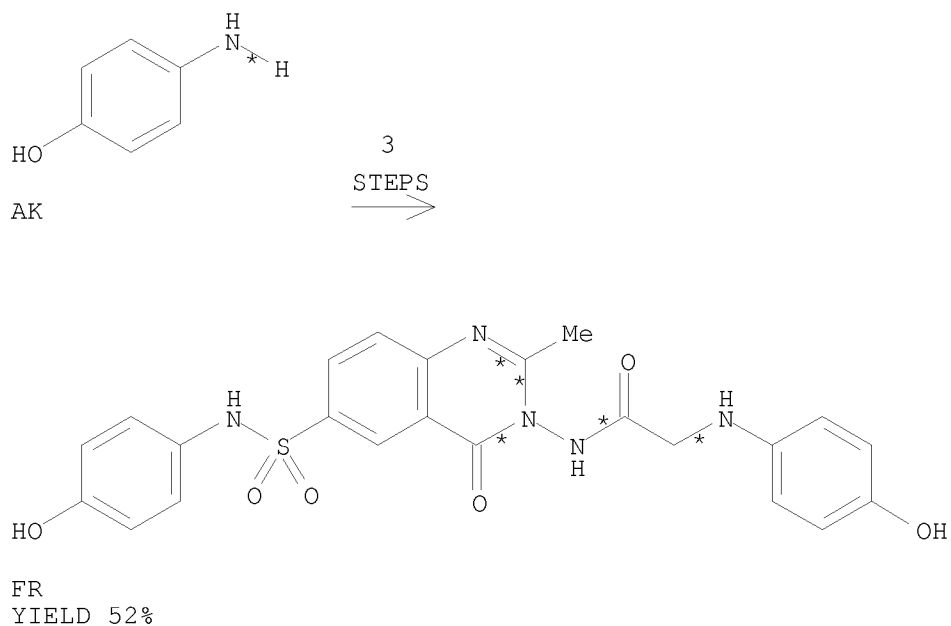


AL



DP

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RX(55) RCT AL 774217-01-5

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CU 774217-38-8  
NTE chemoselective

RX(92) RCT CU 774217-38-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EG 774217-76-4

RX(129) RCT AK 123-30-8, EG 774217-76-4

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH

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CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

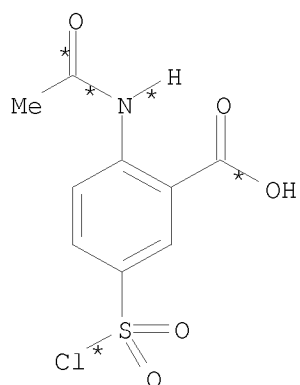
RGT D 7732-18-5 Water

CON cooled

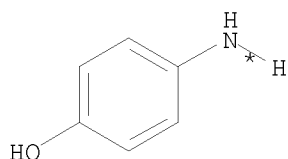
PRO FR 774218-10-9

RX(332) OF 372 COMPOSED OF RX(17), RX(55), RX(92), RX(129)

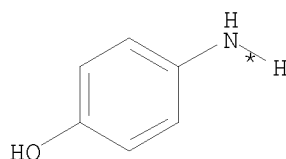
RX(332) A + 2 AK + DP ==> FR



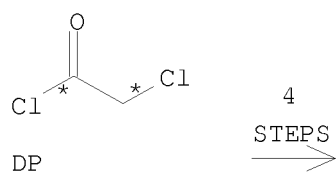
A



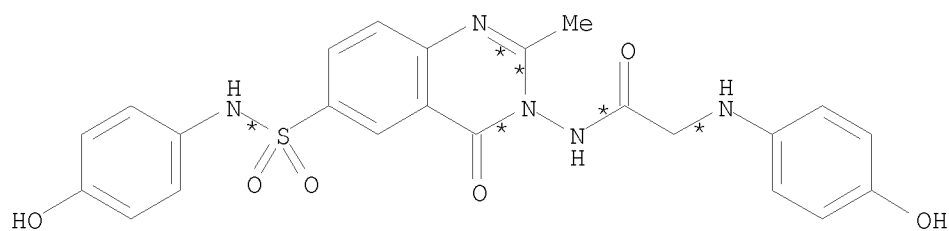
AK



AK



DP



FR  
YIELD 52%

RX(17) RCT A 181478-44-4, AK 123-30-8

STAGE(1)

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CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO AL 774217-01-5

RX(55) RCT AL 774217-01-5

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO CU 774217-38-8  
NTE chemoselective

RX(92) RCT CU 774217-38-8, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EG 774217-76-4

RX(129) RCT AK 123-30-8, EG 774217-76-4

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

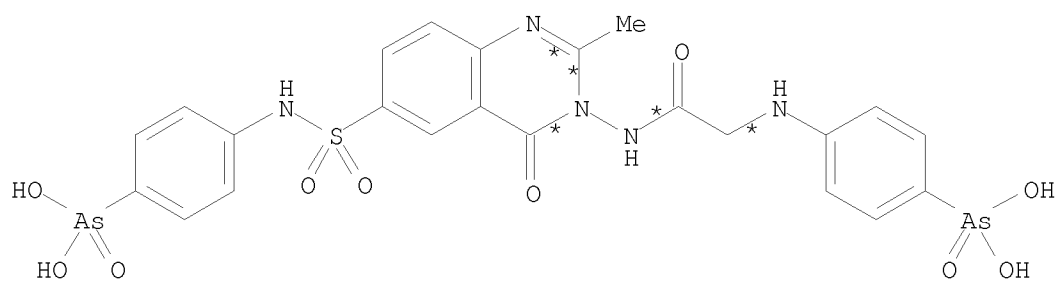
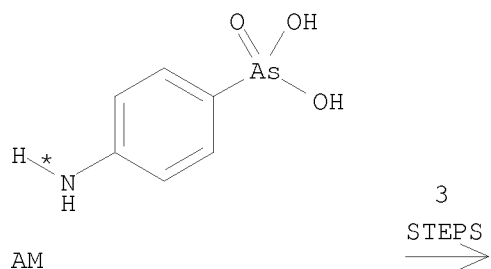
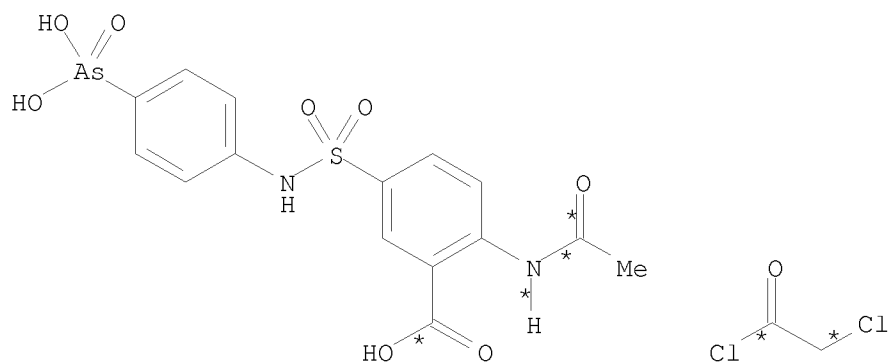
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO FR 774218-10-9

RX(333) OF 372 COMPOSED OF RX(56), RX(93), RX(130)  
RX(333) AN + DP + AM ==> FS



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YIELD 60%

RX(56) RCT AN 774217-02-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

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PRO CV 774217-39-9  
NTE chemoselective

RX(93) RCT CV 774217-39-9, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EH 774217-77-5

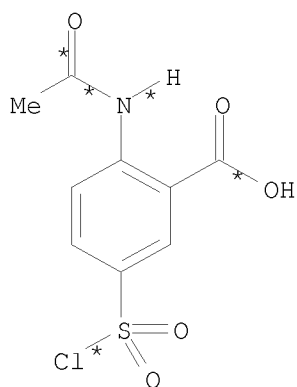
RX(130) RCT AM 98-50-0, EH 774217-77-5

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

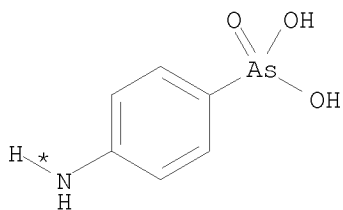
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO FS 774218-11-0

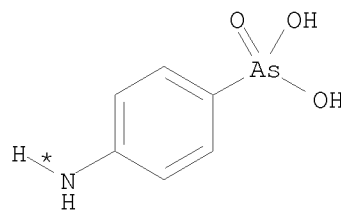
RX(334) OF 372 COMPOSED OF RX(18), RX(56), RX(93), RX(130)  
RX(334) A + 2 AM + DP ==> FS



A

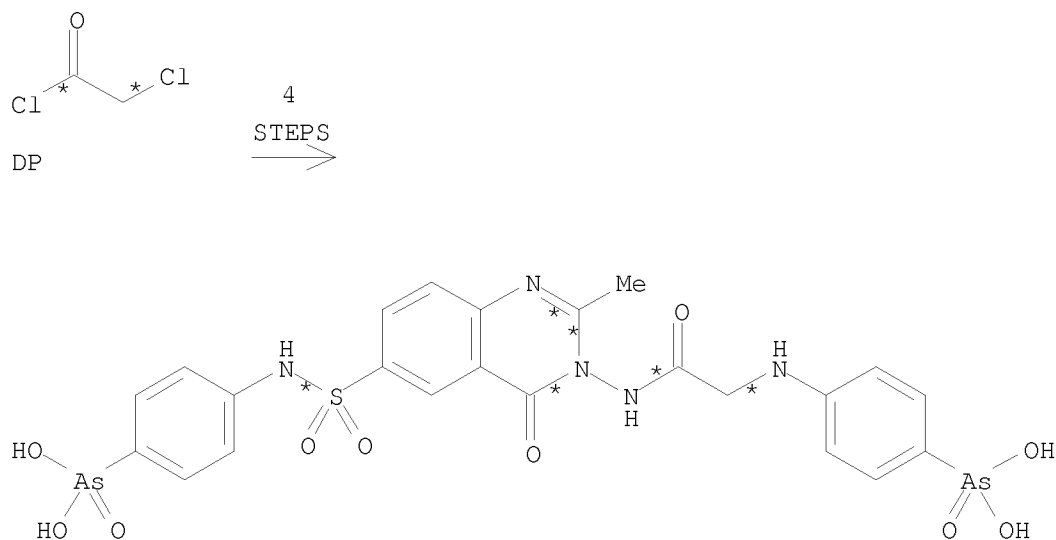


AM



AM

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FS  
YIELD 60%

RX(18) RCT A 181478-44-4, AM 98-50-0

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AN 774217-02-6

RX(56) RCT AN 774217-02-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CV 774217-39-9

NTE chemoselective

RX(93) RCT CV 774217-39-9, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

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SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EH 774217-77-5

RX(130) RCT AM 98-50-0, EH 774217-77-5

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

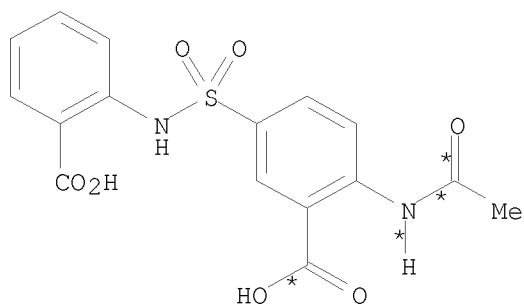
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

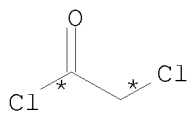
PRO FS 774218-11-0

RX(335) OF 372 COMPOSED OF RX(57), RX(94), RX(131)

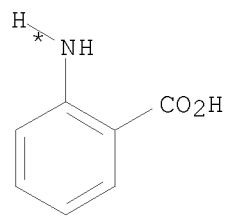
RX(335) AP + DP + AO ==> FT



AP



DP

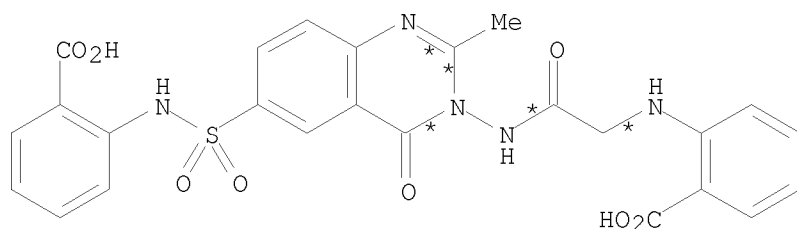


AO

3

STEPS  
→

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FT  
YIELD 63%

RX(57) RCT AP 774217-03-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CW 774217-40-2

NTE chemoselective

RX(94) RCT CW 774217-40-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EI 774217-78-6

RX(131) RCT AO 118-92-3, EI 774217-78-6

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

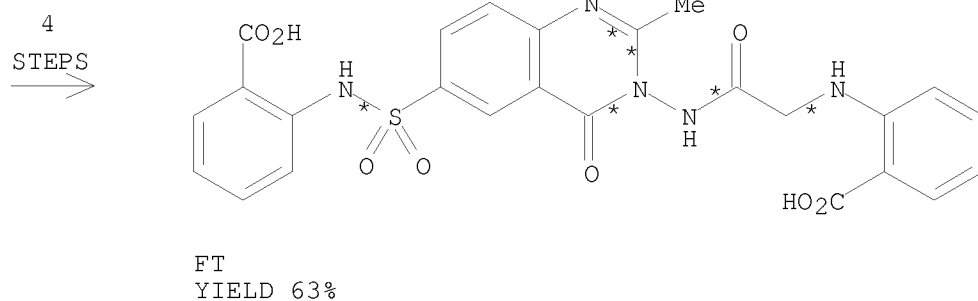
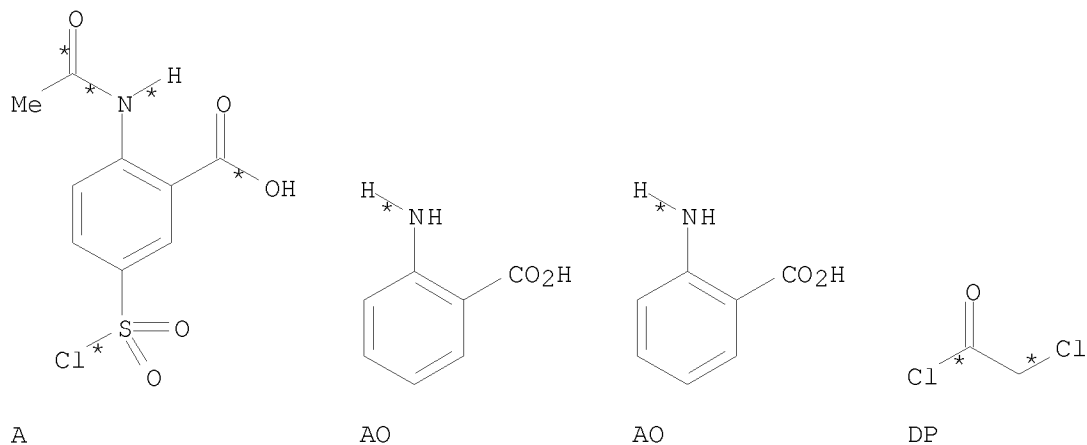
CON cooled

PRO FT 774218-12-1

RX(336) OF 372 COMPOSED OF RX(19), RX(57), RX(94), RX(131)

RX(336) A + 2 AO + DP ==> FT

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RX(19) RCT A 181478-44-4, AO 118-92-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AP 774217-03-7

RX(57) RCT AP 774217-03-7

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

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PRO CW 774217-40-2  
NTE chemoselective

RX(94) RCT CW 774217-40-2, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EI 774217-78-6

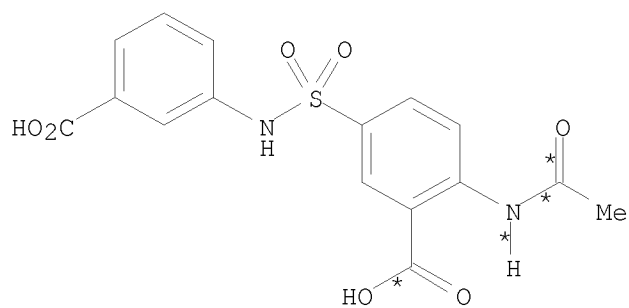
RX(131) RCT AO 118-92-3, EI 774217-78-6

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

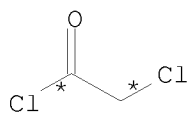
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO FT 774218-12-1

RX(337) OF 372 COMPOSED OF RX(58), RX(95), RX(132)  
RX(337) AR + DP + AQ ==> FU

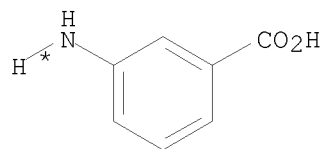


AR



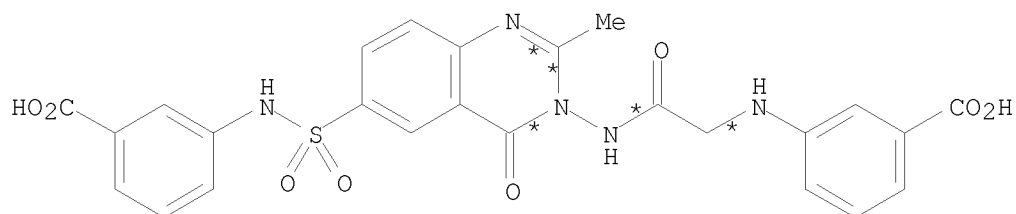
DP

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AQ

3  
STEPS  
→



FU  
YIELD 61%

RX(58) RCT AR 774217-04-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CX 774217-41-3  
NTE chemoselective

RX(95) RCT CX 774217-41-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EJ 774217-79-7

RX(132) RCT AQ 99-05-8, EJ 774217-79-7

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled



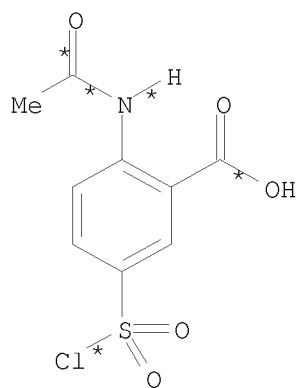
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STAGE(2)

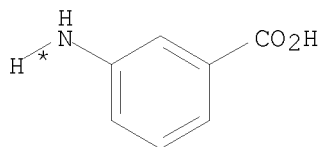
RGT D 7732-18-5 Water  
CON cooled

PRO FU 774218-13-2

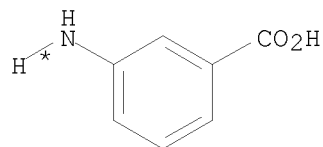
RX(338) OF 372 COMPOSED OF RX(20), RX(58), RX(95), RX(132)  
RX(338) A + 2 AQ + DP ==> FU



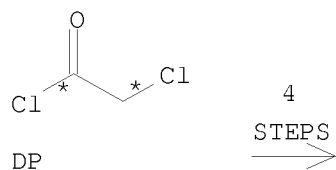
A



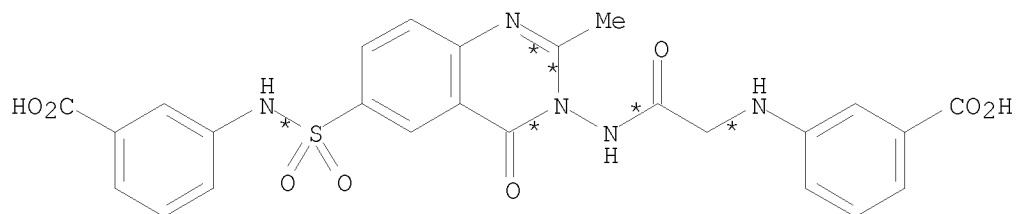
AQ



AQ



4  
STEPS  
→



FU  
YIELD 61%

RX(20) RCT A 181478-44-4, AQ 99-05-8

STAGE(1)

CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH

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CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO AR 774217-04-8

RX(58) RCT AR 774217-04-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CX 774217-41-3  
NTE chemoselective

RX(95) RCT CX 774217-41-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EJ 774217-79-7

RX(132) RCT AQ 99-05-8, EJ 774217-79-7

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

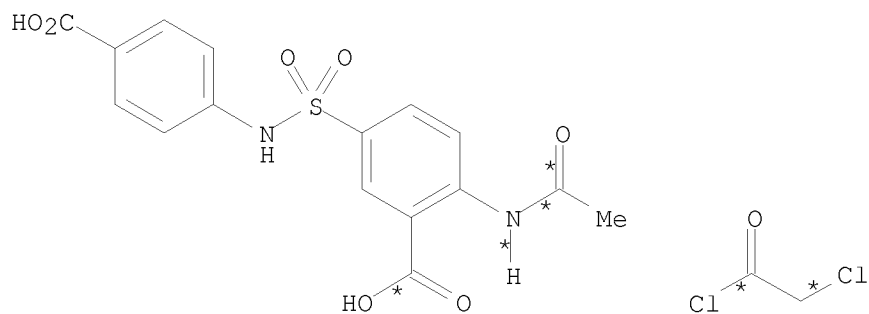
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO FU 774218-13-2

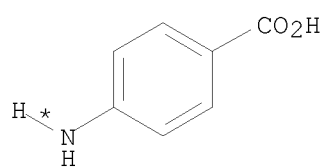
RX(339) OF 372 COMPOSED OF RX(59), RX(96), RX(133)  
RX(339) AT + DP + AS ==> FV

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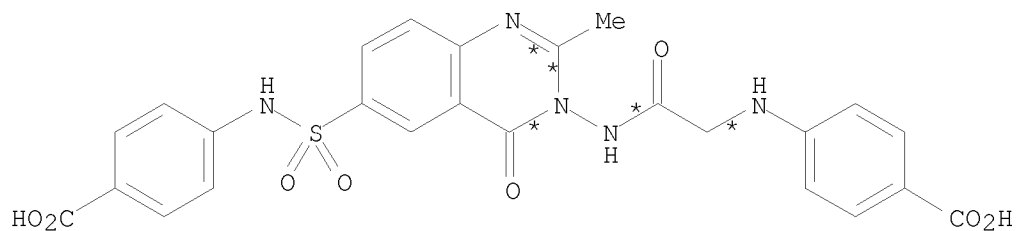
AT

DP



AS

3  
STEPS  
→



FV  
YIELD 63%

RX(59) RCT AT 774217-05-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CY 774217-42-4  
NTE chemoselective

RX(96) RCT CY 774217-42-4, DP 79-04-9

STAGE(1)

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RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EK 774217-80-0

RX(133) RCT AS 150-13-0, EK 774217-80-0

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

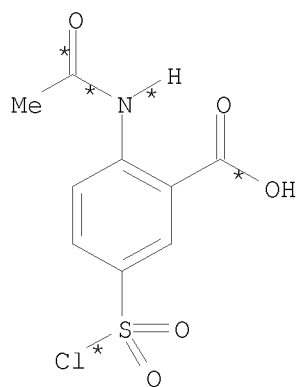
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

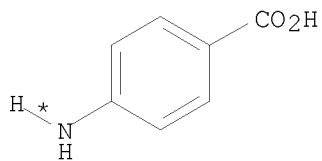
PRO FV 774218-14-3

RX(340) OF 372 COMPOSED OF RX(21), RX(59), RX(96), RX(133)

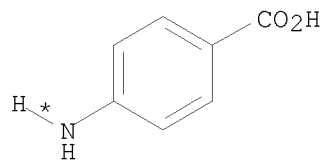
RX(340) A + 2 AS + DP ==> FV



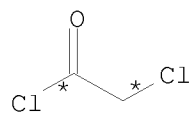
A



AS



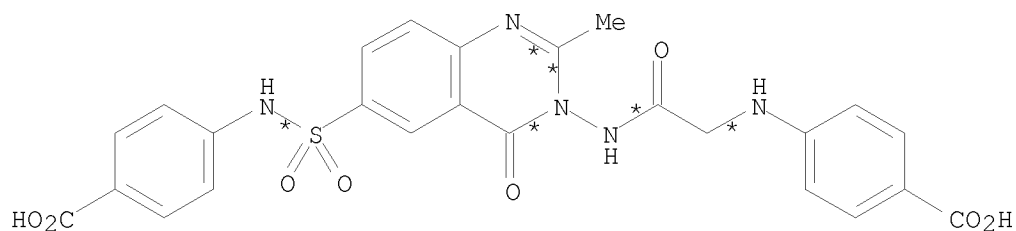
AS



DP

4  
STEPS  
→

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FV  
YIELD 63%

RX(21) RCT A 181478-44-4, AS 150-13-0

STAGE(1)

CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO AT 774217-05-9

RX(59) RCT AT 774217-05-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CY 774217-42-4  
NTE chemoselective

RX(96) RCT CY 774217-42-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EK 774217-80-0

RX(133) RCT AS 150-13-0, EK 774217-80-0

STAGE(1)

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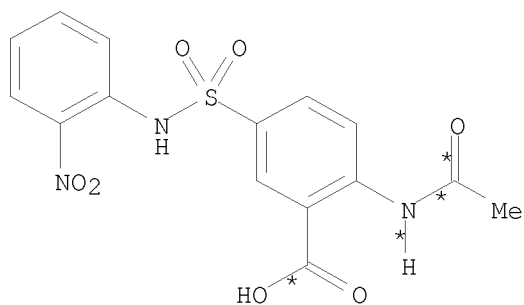
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

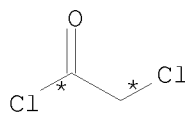
RGT D 7732-18-5 Water  
CON cooled

PRO FV 774218-14-3

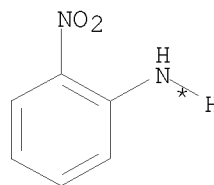
RX(341) OF 372 COMPOSED OF RX(60), RX(97), RX(134)  
RX(341) AV + DP + AU ==> FW



AV

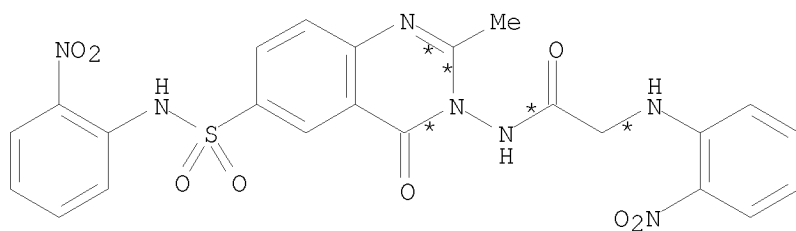


DP



AU

3  
STEPS  
=>



FW  
YIELD 65%

RX(60) RCT AV 774217-06-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

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RGT D 7732-18-5 Water  
CON cooled

PRO CZ 774217-43-5  
NTE chemoselective

RX(97) RCT CZ 774217-43-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EL 774217-81-1

RX(134) RCT AU 88-74-4, EL 774217-81-1

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

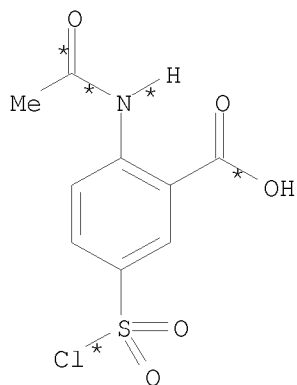
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

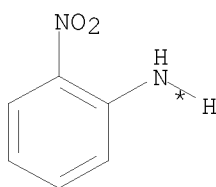
PRO FW 774218-15-4

RX(342) OF 372 COMPOSED OF RX(22), RX(60), RX(97), RX(134)

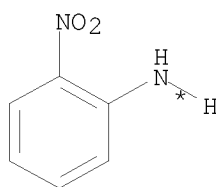
RX(342) A + 2 AU + DP ==> FW



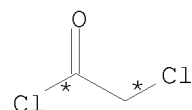
A



AU

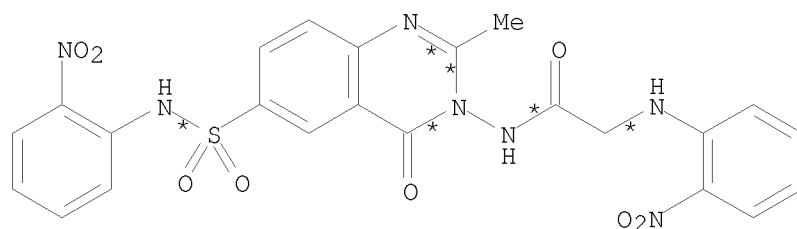


AU



DP

4  
STEPS  
→



FW  
YIELD 65%

RX(22) RCT A 181478-44-4, AU 88-74-4

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AV 774217-06-0

RX(60) RCT AV 774217-06-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CZ 774217-43-5

NTE chemoselective

RX(97) RCT CZ 774217-43-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EL 774217-81-1

RX(134) RCT AU 88-74-4, EL 774217-81-1

STAGE(1)



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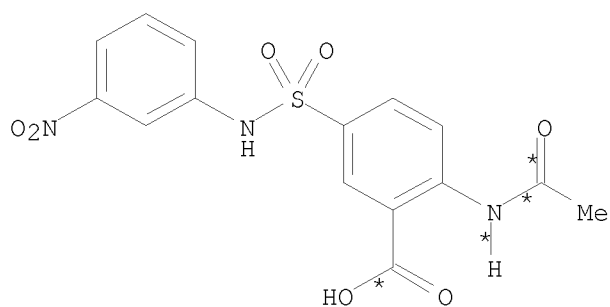
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

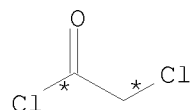
RGT D 7732-18-5 Water  
CON cooled

PRO FW 774218-15-4

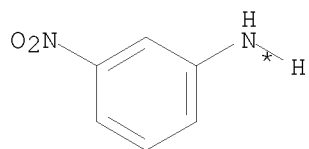
RX(343) OF 372 COMPOSED OF RX(61), RX(98), RX(135)  
RX(343) AX + DP + AW ==> FX



AX

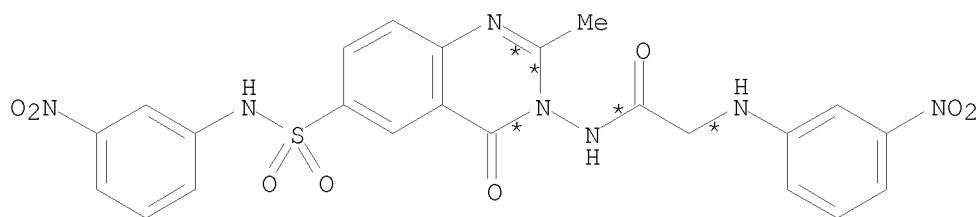


DP



AW

3  
STEPS  
→



FX  
YIELD 63%

RX(61) RCT AX 774217-07-1

STAGE(1)

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RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DA 774217-44-6  
NTE chemoselective

RX(98) RCT DA 774217-44-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EM 774217-82-2

RX(135) RCT AW 99-09-2, EM 774217-82-2

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

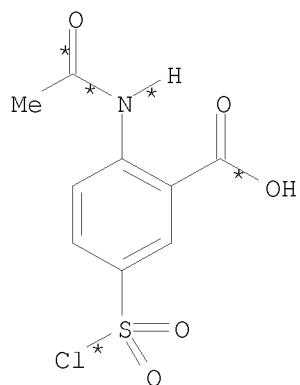
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

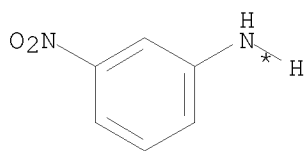
PRO FX 774218-16-5

RX(344) OF 372 COMPOSED OF RX(23), RX(61), RX(98), RX(135)

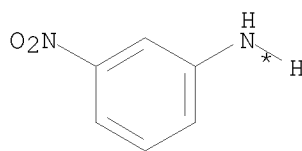
RX(344) A + 2 AW + DP ==> FX



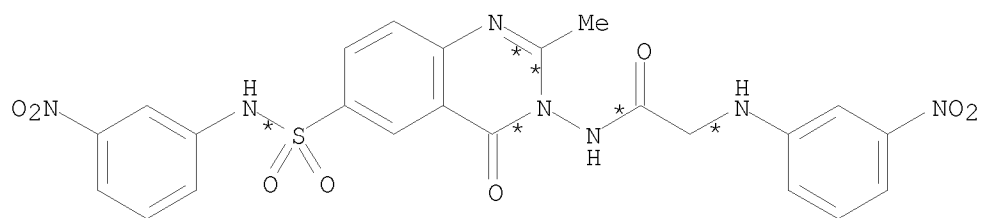
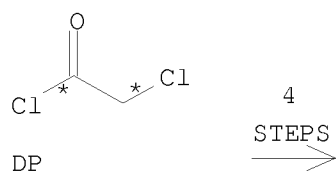
A



AW



AW



FX  
YIELD 63%

RX(23) RCT A 181478-44-4, AW 99-09-2

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AX 774217-07-1

RX(61) RCT AX 774217-07-1

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STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DA 774217-44-6  
NTE chemoselective

RX(98) RCT DA 774217-44-6, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EM 774217-82-2

RX(135) RCT AW 99-09-2, EM 774217-82-2

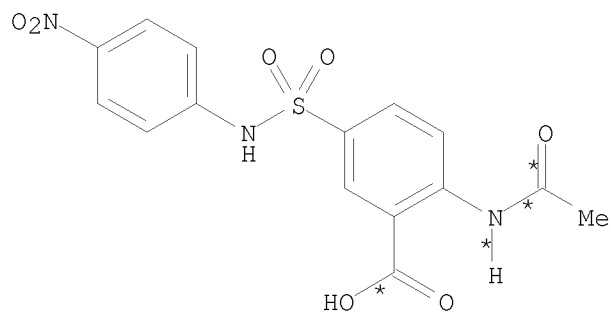
STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

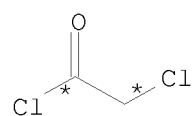
PRO FX 774218-16-5

RX(345) OF 372 COMPOSED OF RX(62), RX(99), RX(136)

RX(345) AZ + DP + AY ==> FY

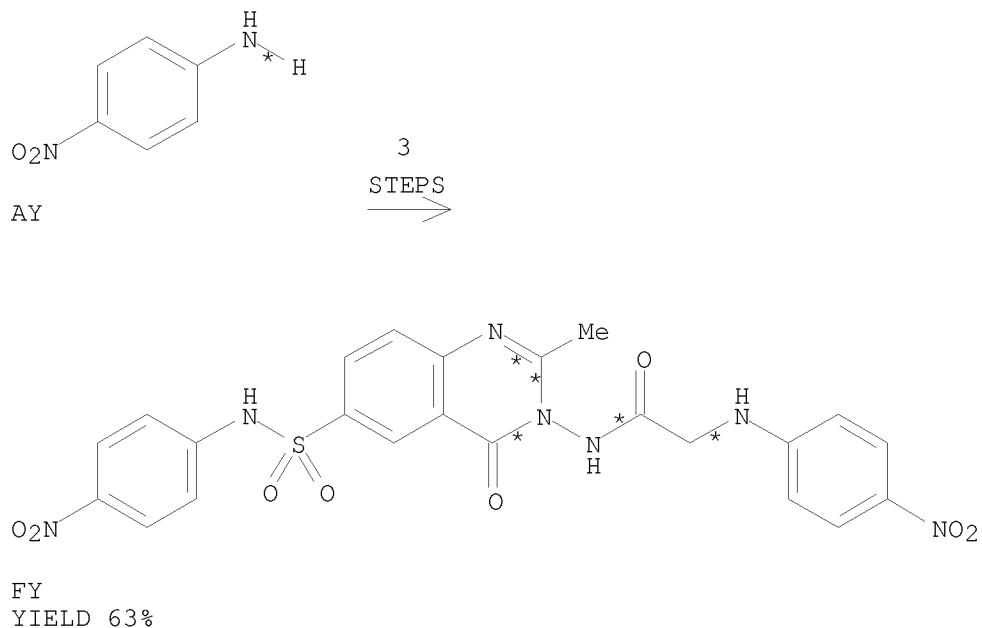


AZ



DP

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RX(62) RCT AZ 774217-08-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DB 774217-45-7

NTE chemoselective

RX(99) RCT DB 774217-45-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EN 774217-83-3

RX(136) RCT AY 100-01-6, EN 774217-83-3

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH

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CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

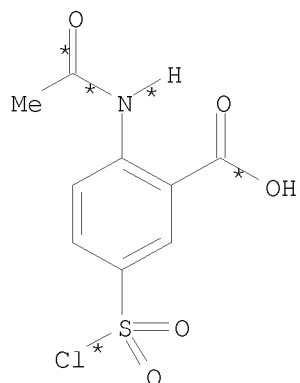
RGT D 7732-18-5 Water

CON cooled

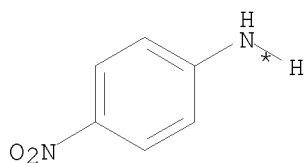
PRO FY 774218-17-6

RX(346) OF 372 COMPOSED OF RX(24), RX(62), RX(99), RX(136)

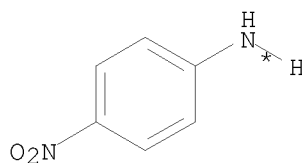
RX(346) A + 2 AY + DP ==> FY



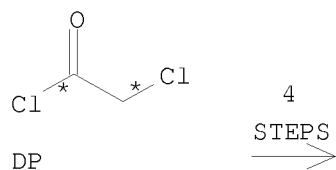
A



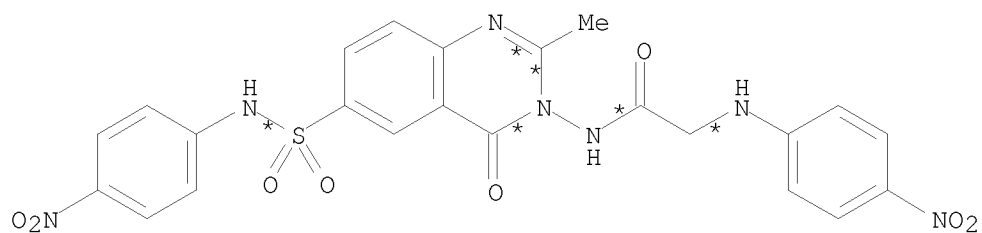
AY



AY



DP



FY

YIELD 63%

RX(24) RCT A 181478-44-4, AY 100-01-6

STAGE(1)

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CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO AZ 774217-08-2

RX(62) RCT AZ 774217-08-2

STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DB 774217-45-7  
NTE chemoselective

RX(99) RCT DB 774217-45-7, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EN 774217-83-3

RX(136) RCT AY 100-01-6, EN 774217-83-3

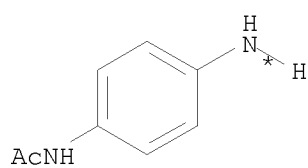
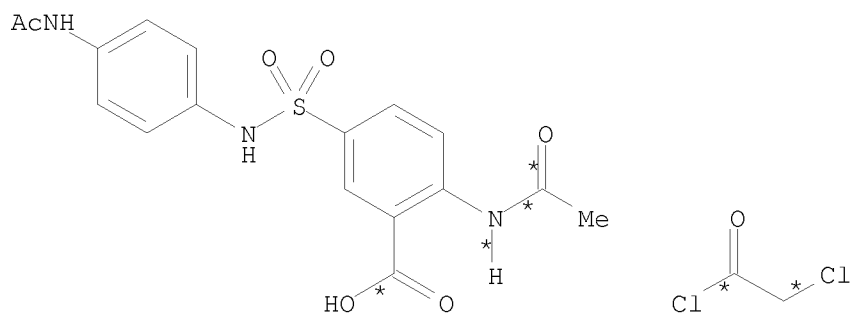
STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

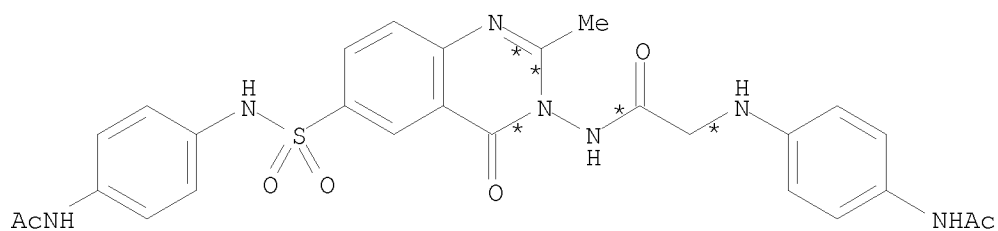
PRO FY 774218-17-6

RX(347) OF 372 COMPOSED OF RX(63), RX(100), RX(137)  
RX(347) BB + DP + BA ==> FZ

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3  
STEPS  
→



YIELD 53%

RX(63) RCT BB 774217-09-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DC 774217-46-8  
NTE chemoselective

RX(100) RCT DC 774217-46-8, DP 79-04-9

STAGE(1)



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RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EO 774217-84-4

RX(137) RCT BA 122-80-5, EO 774217-84-4

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

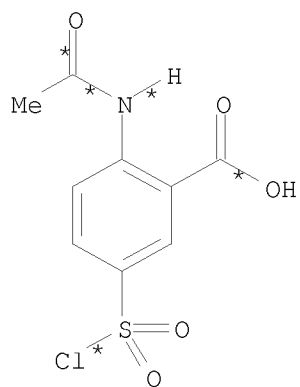
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

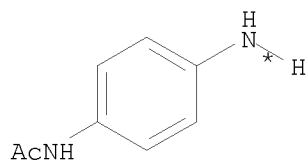
PRO FZ 774218-18-7

RX(348) OF 372 COMPOSED OF RX(25), RX(63), RX(100), RX(137)

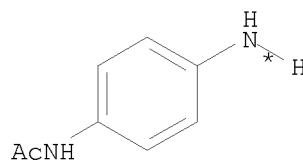
RX(348) A + 2 BA + DP ==> FZ



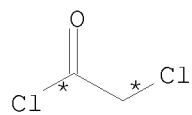
A



BA



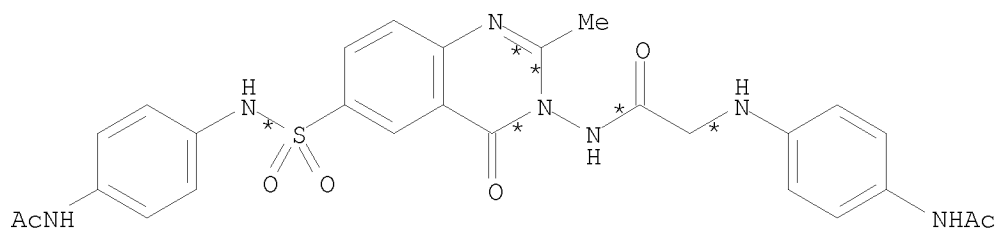
BA



DP

4  
STEPS  
→

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FZ  
YIELD 53%

RX(25) RCT A 181478-44-4, BA 122-80-5

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BB 774217-09-3

RX(63) RCT BB 774217-09-3

STAGE(1)

RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DC 774217-46-8

NTE chemoselective

RX(100) RCT DC 774217-46-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EO 774217-84-4

RX(137) RCT BA 122-80-5, EO 774217-84-4

STAGE(1)

10/ 562,112

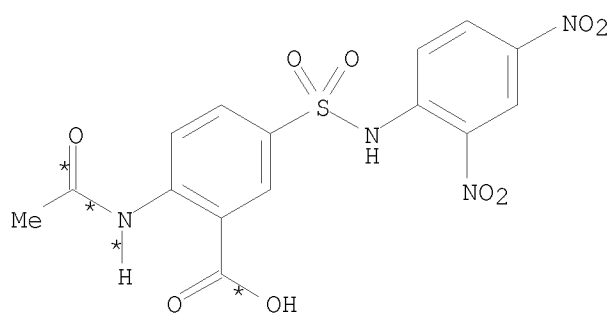
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

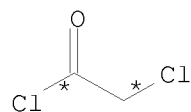
RGT D 7732-18-5 Water  
CON cooled

PRO FZ 774218-18-7

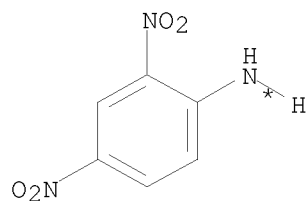
RX(349) OF 372 COMPOSED OF RX(64), RX(101), RX(138)  
RX(349) BD + DP + BC ==> GA



BD

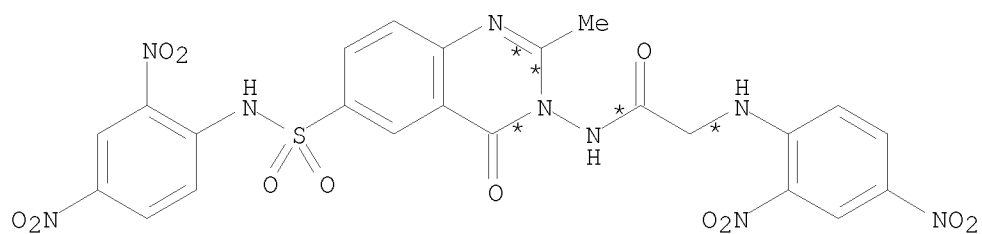


DP



BC

3  
STEPS  
→



GA  
YIELD 61%

10/ 562,112

RX(64) RCT BD 774217-10-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DD 774217-47-9

NTE chemoselective

RX(101) RCT DD 774217-47-9, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EP 774217-85-5

RX(138) RCT BC 97-02-9, EP 774217-85-5

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

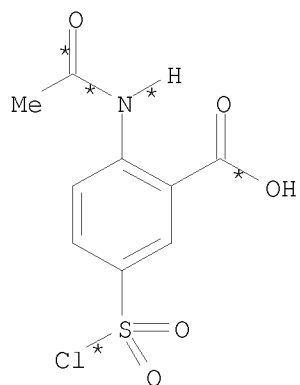
RGT D 7732-18-5 Water

CON cooled

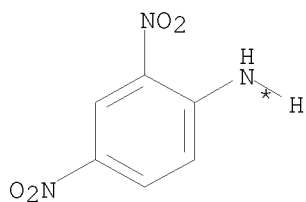
PRO GA 774218-19-8

RX(350) OF 372 COMPOSED OF RX(26), RX(64), RX(101), RX(138)

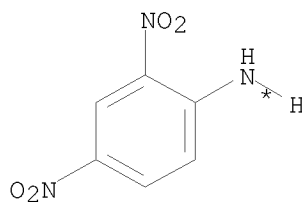
RX(350) A + 2 BC + DP ==> GA



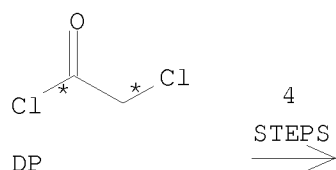
A



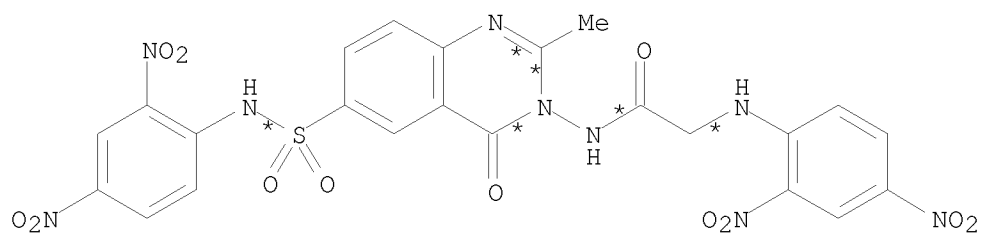
BC



BC



DP



GA

YIELD 61%

RX(26) RCT A 181478-44-4, BC 97-02-9

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BD 774217-10-6

RX(64) RCT BD 774217-10-6

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STAGE(1)  
RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DD 774217-47-9  
NTE chemoselective

RX(101) RCT DD 774217-47-9, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EP 774217-85-5

RX(138) RCT BC 97-02-9, EP 774217-85-5

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

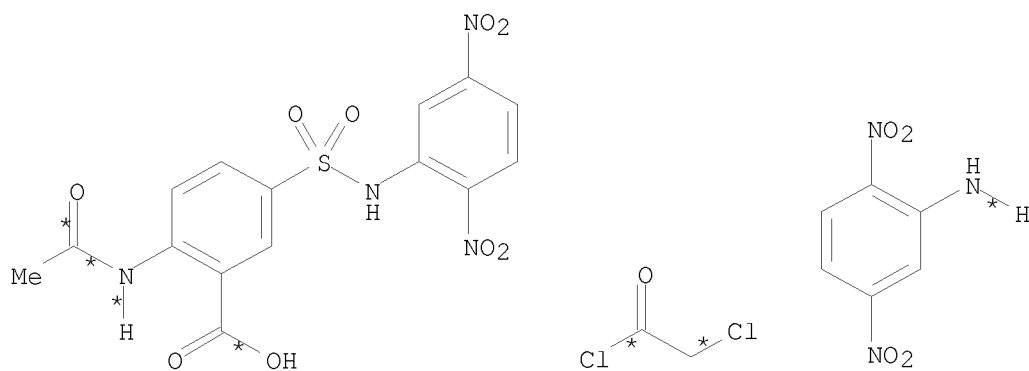
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO GA 774218-19-8

RX(351) OF 372 COMPOSED OF RX(65), RX(102), RX(139)

RX(351) BF + DP + BE ==> GB

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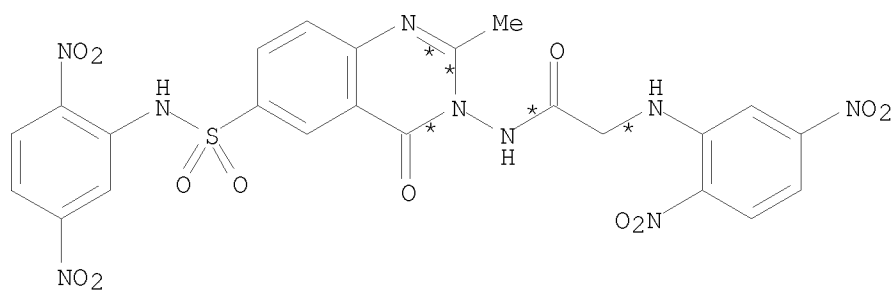


BF

DP

BE

3  
STEPS  
→



GB  
YIELD 63%

RX(65) RCT BF 774217-11-7

STAGE(1)  
RGT CD 7803-57-8 N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO DE 774217-48-0  
NTE chemoselective

RX(102) RCT DE 774217-48-0, DP 79-04-9

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH

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CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EQ 774217-86-6

RX(139) RCT BE 619-18-1, EQ 774217-86-6

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

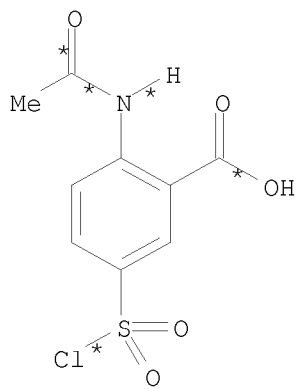
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

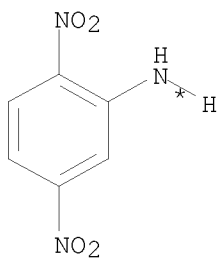
PRO GB 774218-20-1

RX(352) OF 372 COMPOSED OF RX(27), RX(65), RX(102), RX(139)

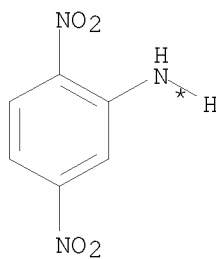
RX(352) A + 2 BE + DP ==> GB



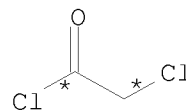
A



BE



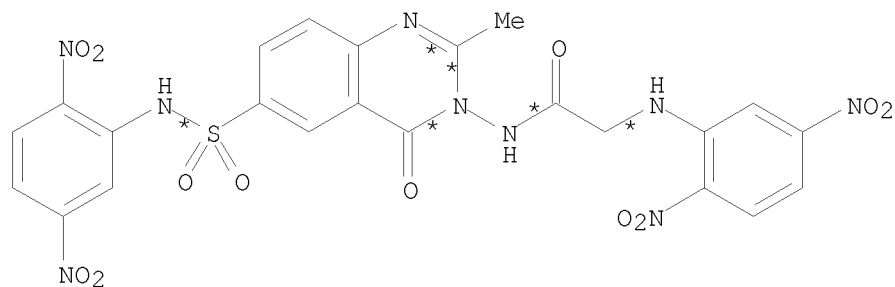
BE



DP



4  
STEPS  
→



GB  
YIELD 63%

RX(27) RCT A 181478-44-4, BE 619-18-1

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BF 774217-11-7

RX(65) RCT BF 774217-11-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DE 774217-48-0

NTE chemoselective

RX(102) RCT DE 774217-48-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EQ 774217-86-6

RX(139) RCT BE 619-18-1, EQ 774217-86-6

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STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

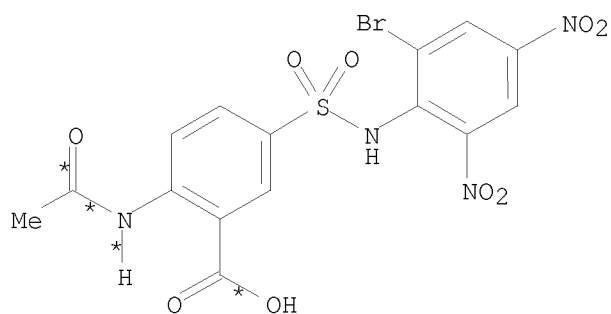
RGT D 7732-18-5 Water

CON cooled

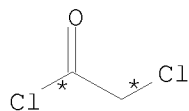
PRO GB 774218-20-1

RX(353) OF 372 COMPOSED OF RX(66), RX(103), RX(140)

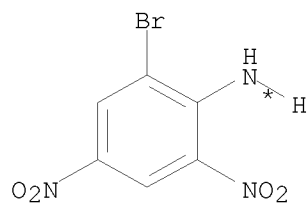
RX(353) BH + DP + BG ==> GC



BH

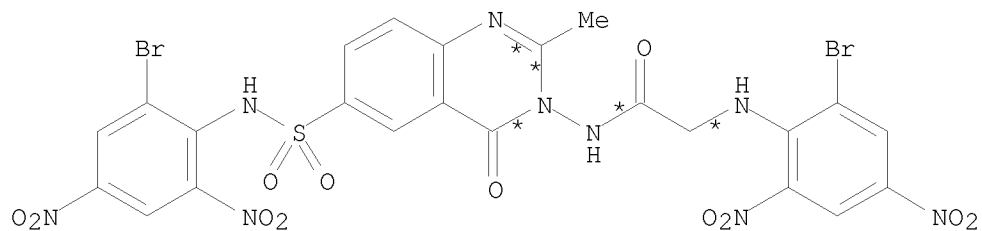


DP



BG

3  
STEPS  
→



GC

YIELD 63%

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RX(66) RCT BH 774217-12-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DF 774217-49-1

NTE chemoselective

RX(103) RCT DF 774217-49-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO ER 774217-87-7

RX(140) RCT BG 1817-73-8, ER 774217-87-7

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

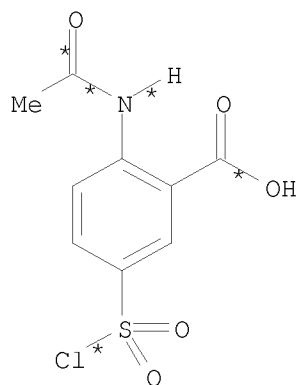
RGT D 7732-18-5 Water

CON cooled

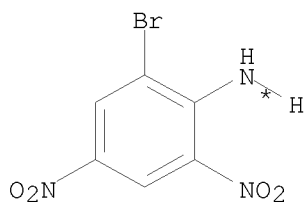
PRO GC 774218-21-2

RX(354) OF 372 COMPOSED OF RX(28), RX(66), RX(103), RX(140)

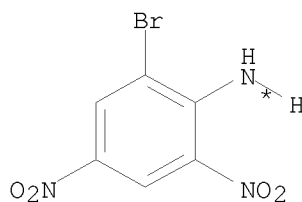
RX(354) A + 2 BG + DP ==> GC



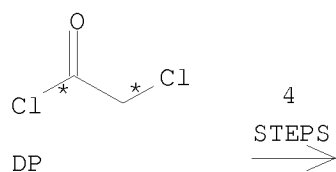
A



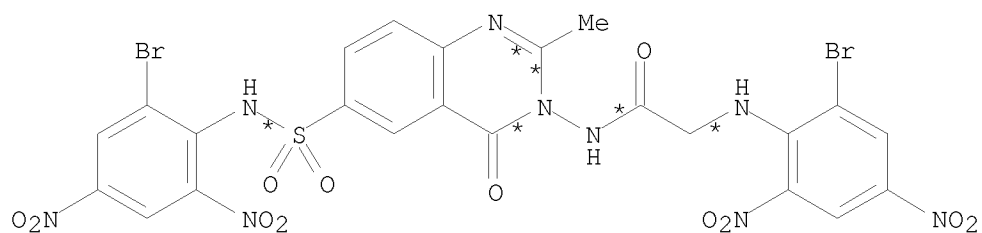
BG



BG



DP



GC

YIELD 63%

RX(28) RCT A 181478-44-4, BG 1817-73-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BH 774217-12-8

RX(66) RCT BH 774217-12-8

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STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DF 774217-49-1  
NTE chemoselective

RX(103) RCT DF 774217-49-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO ER 774217-87-7

RX(140) RCT BG 1817-73-8, ER 774217-87-7

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

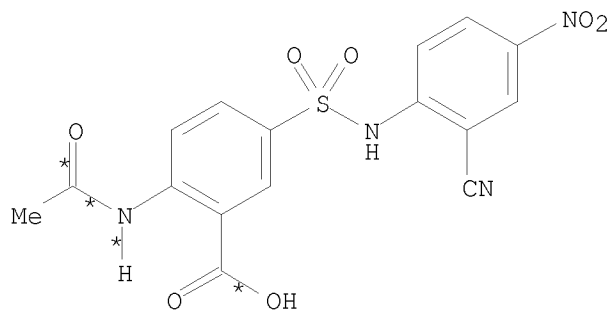
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

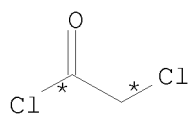
PRO GC 774218-21-2

RX(355) OF 372 COMPOSED OF RX(67), RX(104), RX(141)

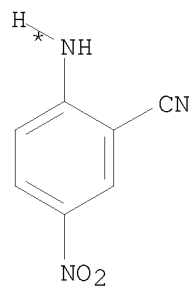
RX(355) BJ + DP + BI ==> GD



BJ



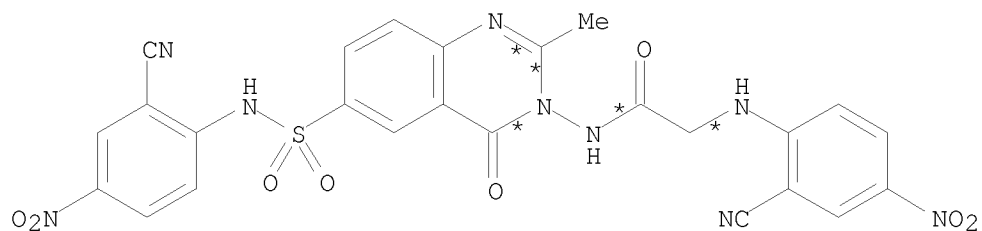
DP



BI

10/ 562,112

3  
STEPS  
→



GD  
YIELD 60%

RX(67) RCT BJ 774217-13-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DG 774217-50-4  
NTE chemoselective

RX(104) RCT DG 774217-50-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO ES 774217-88-8

RX(141) RCT BI 17420-30-3, ES 774217-88-8

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

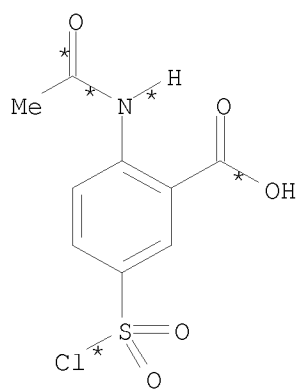
10/ 562,112

CON cooled

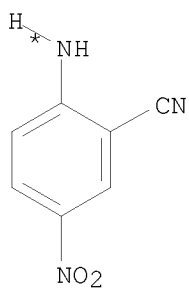
PRO GD 774218-22-3

RX(356) OF 372 COMPOSED OF RX(29), RX(67), RX(104), RX(141)

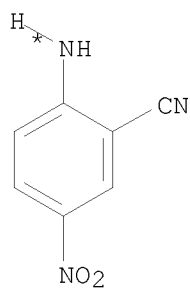
RX(356) A + 2 BI + DP ==> GD



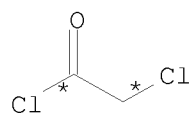
A



BI

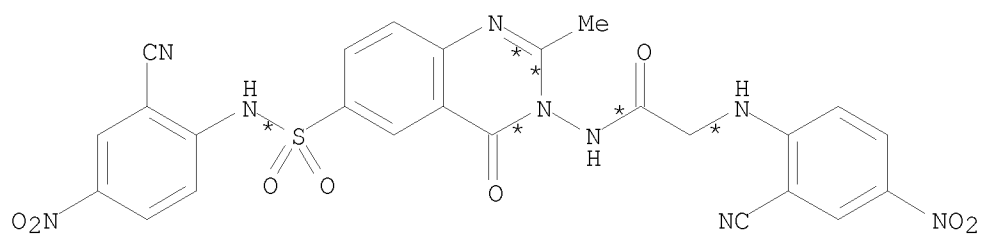


BI



DP

4  
STEPS  
→



GD  
YIELD 60%

RX(29) RCT A 181478-44-4, BI 17420-30-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

10/ 562,112

PRO BJ 774217-13-9

RX(67) RCT BJ 774217-13-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DG 774217-50-4

NTE chemoselective

RX(104) RCT DG 774217-50-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO ES 774217-88-8

RX(141) RCT BI 17420-30-3, ES 774217-88-8

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

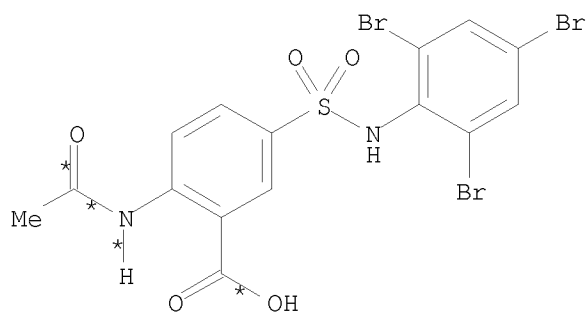
PRO GD 774218-22-3

RX(357) OF 372 COMPOSED OF RX(68), RX(105), RX(142)

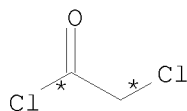
RX(357) BL + DP + BK ==> GE



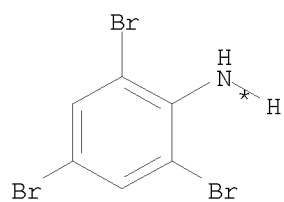
10/ 562,112



BL

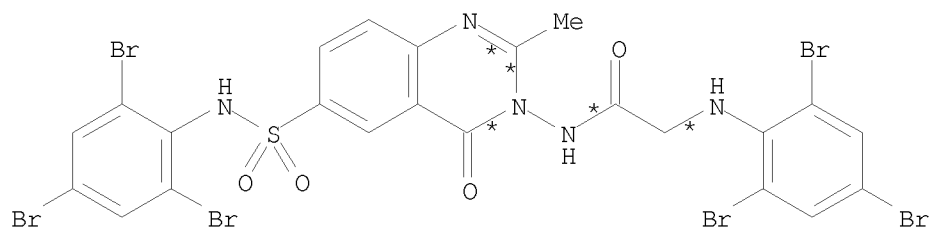


DP



BK

3  
STEPS  
→



GE  
YIELD 65%

RX(68) RCT BL 774217-14-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DH 774217-51-5

NTE chemoselective

RX(105) RCT DH 774217-51-5, DP 79-04-9

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STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO ET 774217-89-9

RX(142) RCT BK 147-82-0, ET 774217-89-9

STAGE(1)

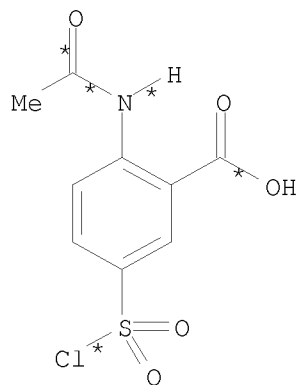
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

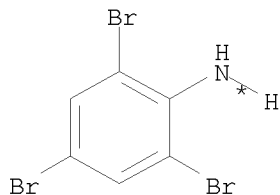
RGT D 7732-18-5 Water  
CON cooled

PRO GE 774218-23-4

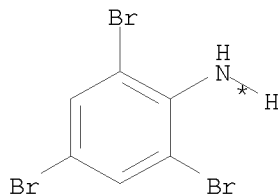
RX(358) OF 372 COMPOSED OF RX(30), RX(68), RX(105), RX(142)  
RX(358) A + 2 BK + DP ==> GE



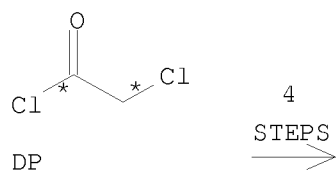
A



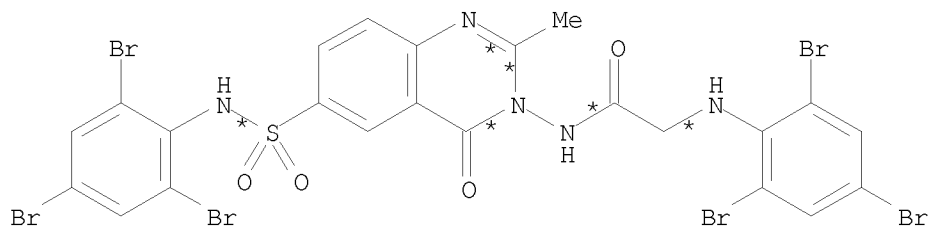
BK



BK



10/ 562,112



GE  
YIELD 65%

RX(30) RCT A 181478-44-4, BK 147-82-0

STAGE (1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE (1) 4 hours, 120 deg C

SUBSTAGE (2) cooled

STAGE (2)

RGT D 7732-18-5 Water

CON    cooled

PRO BL 774217-14-0

RX (68) RCT BL 774217-14-0

STAGE (1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE (2)

RGT D 7732-18-5 Water

CON    cooled

PRO DH 774217-51-5

NTE chemoselective

RX(105) RCT DH 774217-51-5, DP 79-04-9

STAGE (1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE (2) cooled

STAGE (2)

RGT D 7732-18-5 Water

CON    cooled

PRO ET 774217-89-9

RX(142) RCT BK 147-82-0, ET 774217-89-9

STAGE (1)

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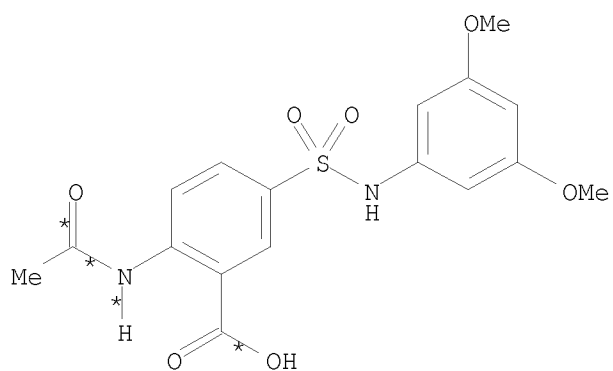
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

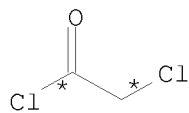
RGT D 7732-18-5 Water  
CON cooled

PRO GE 774218-23-4

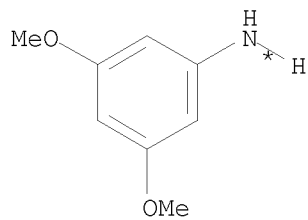
RX(359) OF 372 COMPOSED OF RX(69), RX(106), RX(143)  
RX(359) BN + DP + BM ==> GF



BN



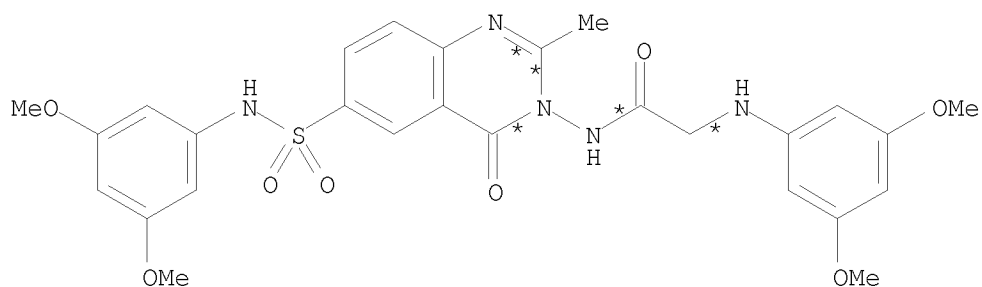
DP



BM

3  
STEPS  
→

10/ 562,112



GF  
YIELD 59%

RX(69) RCT BN 774217-15-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DI 774217-52-6

NTE chemoselective

RX(106) RCT DI 774217-52-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EU 774217-90-2

RX(143) RCT BM 10272-07-8, EU 774217-90-2

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

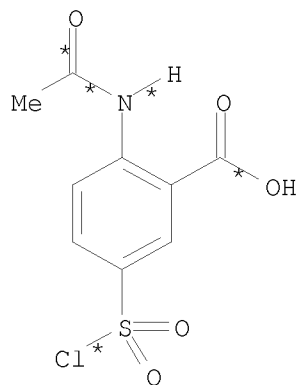
RGT D 7732-18-5 Water

CON cooled

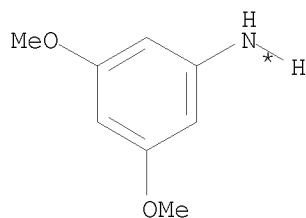
PRO GF 774218-24-5

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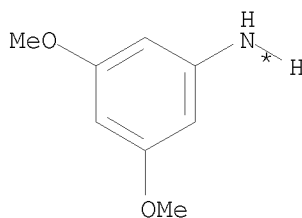
RX(360) OF 372 COMPOSED OF RX(31), RX(69), RX(106), RX(143)  
RX(360) A + 2 BM + DP ==> GF



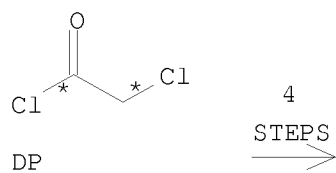
A



BM



BM



GF  
YIELD 59%

RX(31) RCT A 181478-44-4, BM 10272-07-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

10/ 562,112

PRO BN 774217-15-1

RX(69) RCT BN 774217-15-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DI 774217-52-6

NTE chemoselective

RX(106) RCT DI 774217-52-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EU 774217-90-2

RX(143) RCT BM 10272-07-8, EU 774217-90-2

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

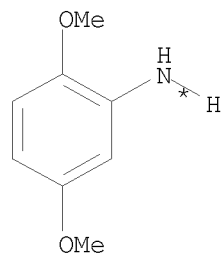
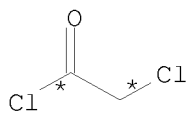
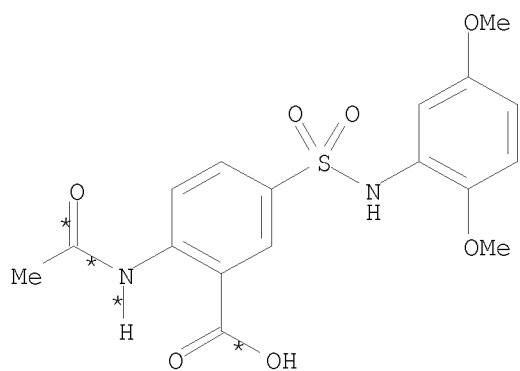
CON cooled

PRO GF 774218-24-5

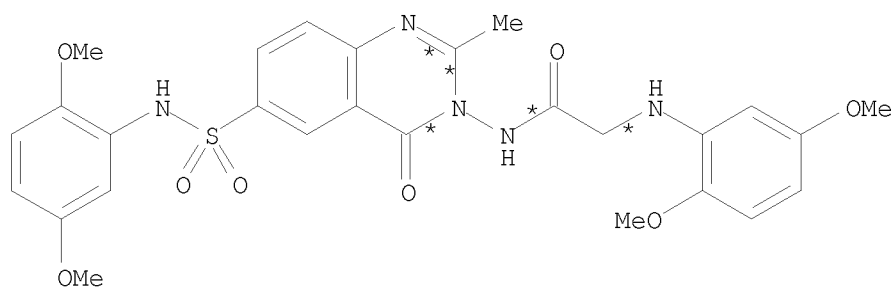
RX(361) OF 372 COMPOSED OF RX(70), RX(107), RX(144)

RX(361) BP + DP + BO ==> GG

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3  
STEPS  
→



YIELD 60%

RX(70) RCT BP 774217-16-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DJ 774217-53-7

NTE chemoselective

RX(107) RCT DJ 774217-53-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH



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CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EV 774217-91-3

RX(144) RCT BO 102-56-7, EV 774217-91-3

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

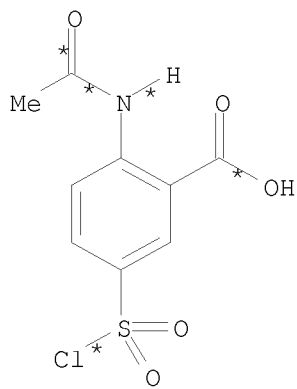
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

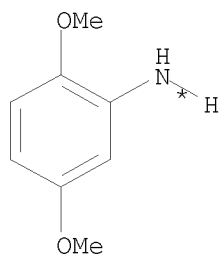
PRO GG 774218-25-6

RX(362) OF 372 COMPOSED OF RX(32), RX(70), RX(107), RX(144)

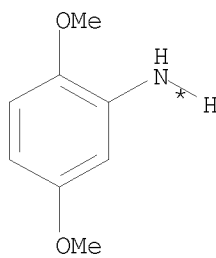
RX(362) A + 2 BO + DP ==> GG



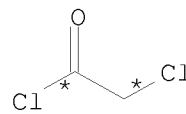
A



BO

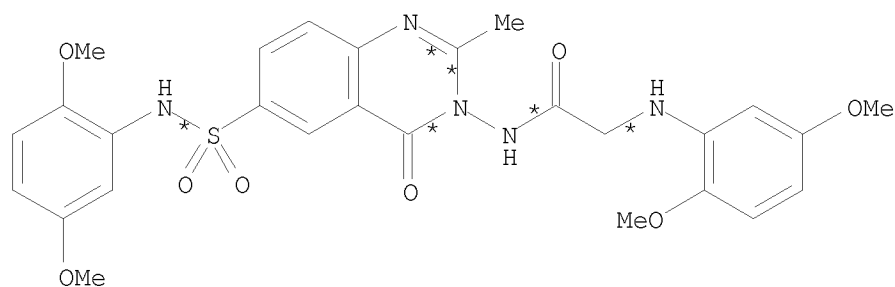


BO



DP

4  
STEPS  
→



GG  
YIELD 60%

RX(32) RCT A 181478-44-4, BO 102-56-7

STAGE(1)

CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO BP 774217-16-2

RX(70) RCT BP 774217-16-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DJ 774217-53-7

NTE chemoselective

RX(107) RCT DJ 774217-53-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO EV 774217-91-3

RX(144) RCT BO 102-56-7, EV 774217-91-3

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STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

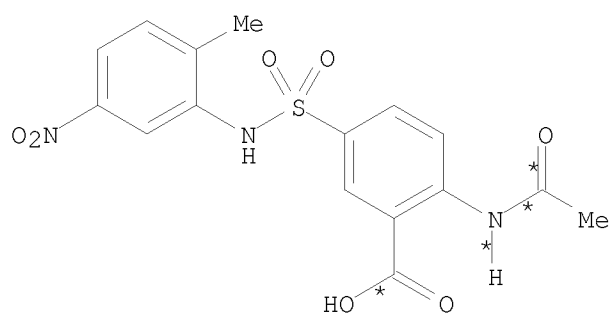
RGT D 7732-18-5 Water

CON cooled

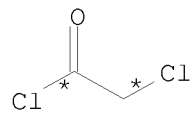
PRO GG 774218-25-6

RX(363) OF 372 COMPOSED OF RX(71), RX(108), RX(145)

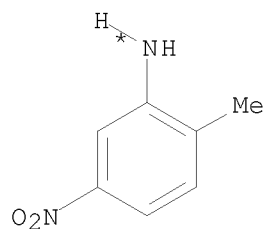
RX(363) BR + DP + BQ ==> GH



BR



DP



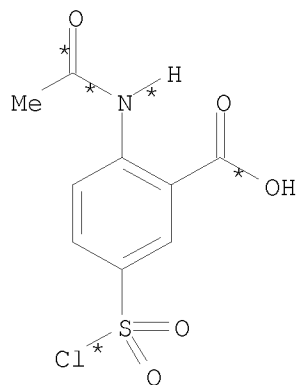
BQ

3  
STEPS  
→

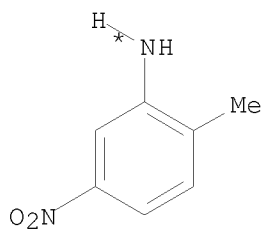


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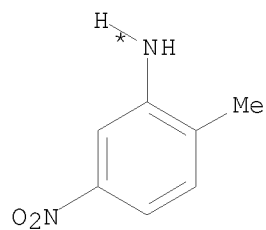
RX(364) OF 372 COMPOSED OF RX(33), RX(71), RX(108), RX(145)  
RX(364) A + 2 BQ + DP ==> GH



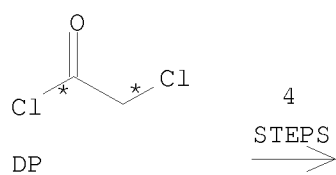
A



BQ

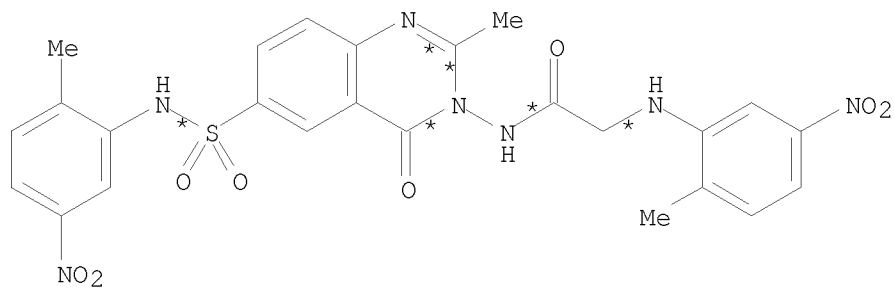


BQ



DP

4  
STEPS  
→



GH  
YIELD 60%

RX(33) RCT A 181478-44-4, BQ 99-55-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

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PRO BR 774217-17-3

RX(71) RCT BR 774217-17-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DK 774217-54-8

NTE chemoselective

RX(108) RCT DK 774217-54-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EW 774217-92-4

RX(145) RCT BQ 99-55-8, EW 774217-92-4

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

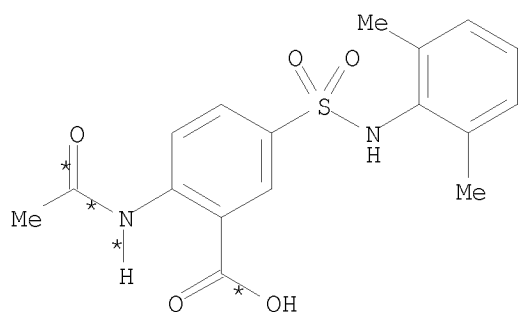
CON cooled

PRO GH 774218-26-7

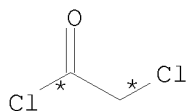
RX(365) OF 372 COMPOSED OF RX(72), RX(109), RX(147)

RX(365) BV + DP + BU ==> GK

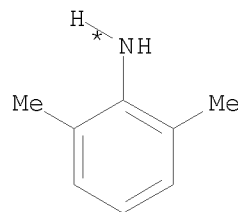
10/ 562,112



BV

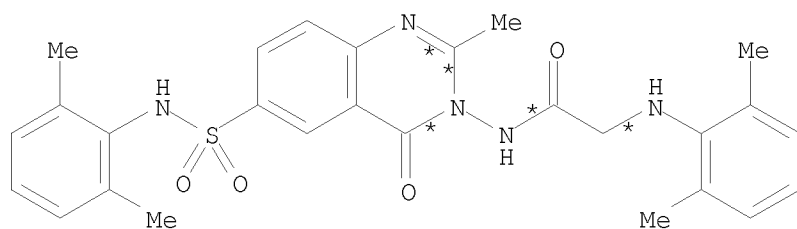


DP



BU

3  
STEPS  
→



GK  
YIELD 57%

RX(72) RCT BV 774217-19-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DL 774217-56-0

NTE chemoselective

RX(109) RCT DL 774217-56-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

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RGT D 7732-18-5 Water  
CON cooled

PRO EX 774217-94-6

RX(147) RCT BU 87-62-7, EX 774217-94-6

STAGE(1)

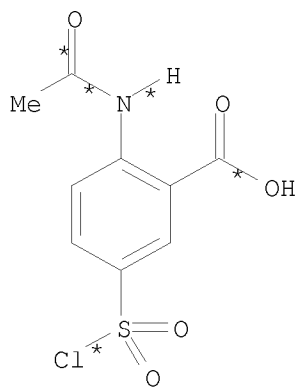
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

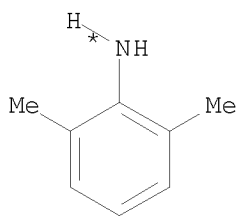
RGT D 7732-18-5 Water  
CON cooled

PRO GK 774218-28-9

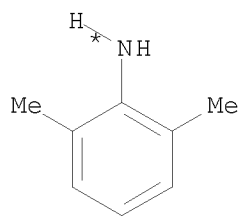
RX(366) OF 372 COMPOSED OF RX(35), RX(72), RX(109), RX(147)  
RX(366) A + 2 BU + DP ==> GK



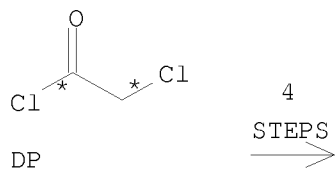
A



BU

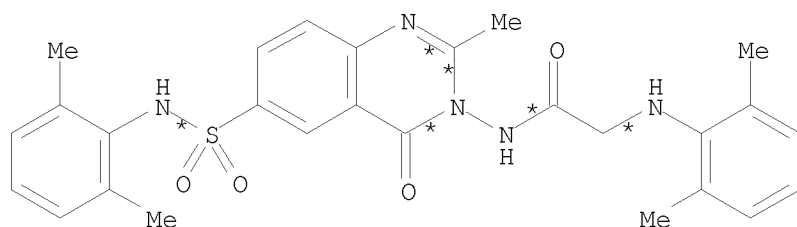


BU





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GK  
YIELD 57%

RX(35) RCT A 181478-44-4, BU 87-62-7

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BV 774217-19-5

RX(72) RCT BV 774217-19-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DL 774217-56-0

NTE chemoselective

RX(109) RCT DL 774217-56-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EX 774217-94-6

RX(147) RCT BU 87-62-7, EX 774217-94-6

STAGE(1)

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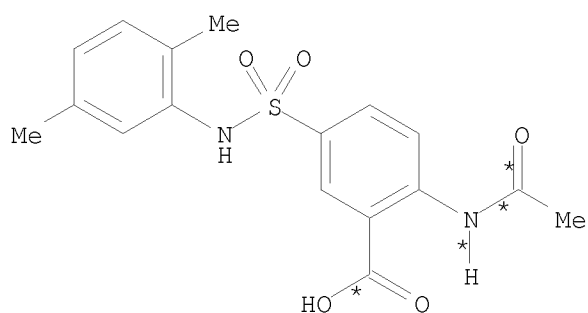
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

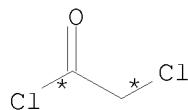
RGT D 7732-18-5 Water  
CON cooled

PRO GK 774218-28-9

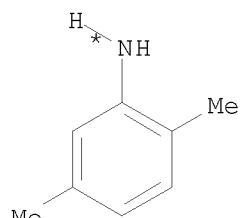
RX(367) OF 372 COMPOSED OF RX(73), RX(110), RX(148)  
RX(367) BX + DP + BW ==> GL



BX



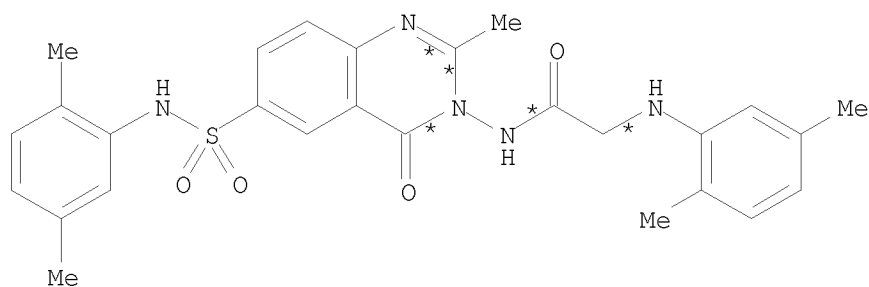
DP



BW

3  
STEPS  
→

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GL  
YIELD 53%

RX(73) RCT BX 774217-20-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DM 774217-57-1

NTE chemoselective

RX(110) RCT DM 774217-57-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EY 774217-95-7

RX(148) RCT BW 95-78-3, EY 774217-95-7

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

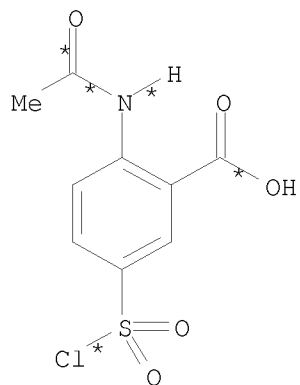
RGT D 7732-18-5 Water

CON cooled

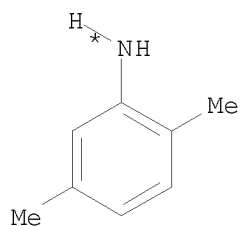
PRO GL 774218-29-0

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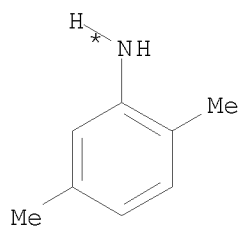
RX(368) OF 372 COMPOSED OF RX(36), RX(73), RX(110), RX(148)  
RX(368) A + 2 BW + DP ==> GL



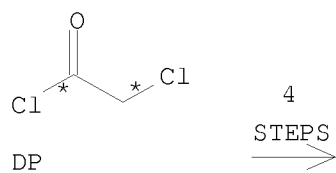
A



BW



BW



GL  
YIELD 53%

RX(36) RCT A 181478-44-4, BW 95-78-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

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PRO BX 774217-20-8

RX(73) RCT BX 774217-20-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DM 774217-57-1

NTE chemoselective

RX(110) RCT DM 774217-57-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EY 774217-95-7

RX(148) RCT BW 95-78-3, EY 774217-95-7

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

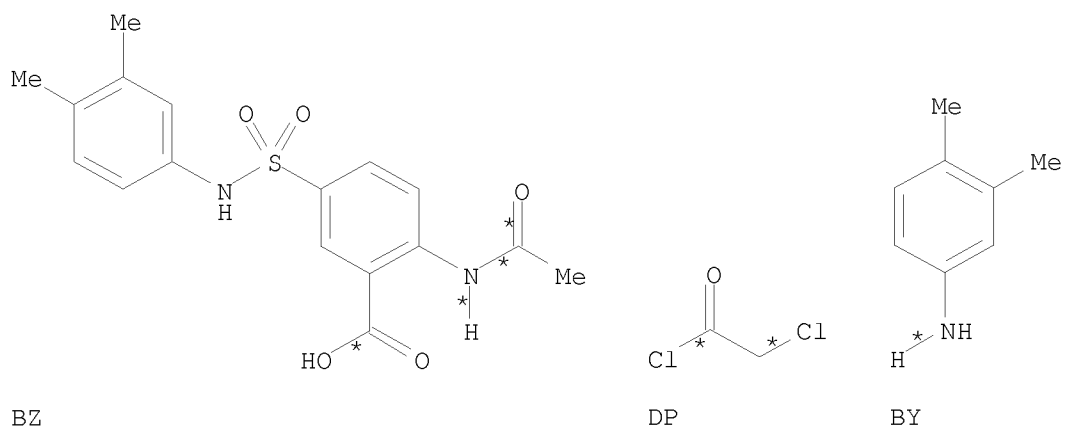
CON cooled

PRO GL 774218-29-0

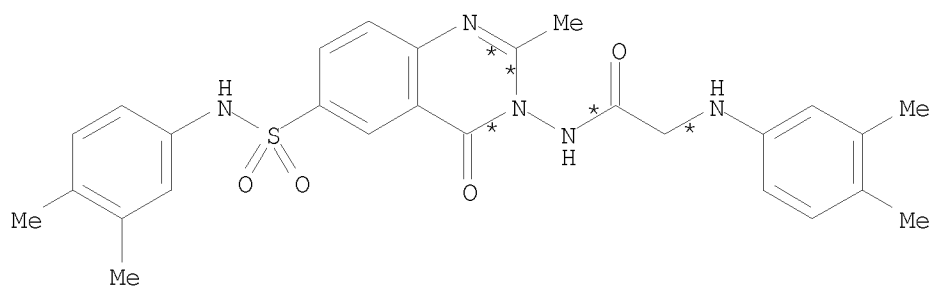
RX(369) OF 372 COMPOSED OF RX(74), RX(111), RX(149)

RX(369) BZ + DP + BY ==> GM

10/ 562,112



3  
STEPS  
→



GM  
YIELD 53%

RX(74) RCT BZ 774217-21-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DN 774217-58-2

NTE chemoselective

RX(111) RCT DN 774217-58-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

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SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO EZ 774217-96-8

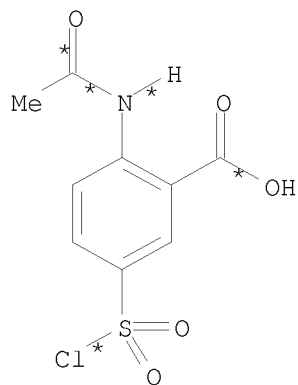
RX(149) RCT BY 95-64-7, EZ 774217-96-8

STAGE(1)  
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

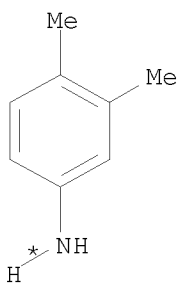
STAGE(2)  
RGT D 7732-18-5 Water  
CON cooled

PRO GM 774218-30-3

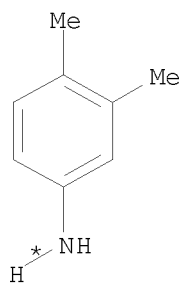
RX(370) OF 372 COMPOSED OF RX(37), RX(74), RX(111), RX(149)  
RX(370) A + 2 BY + DP ==> GM



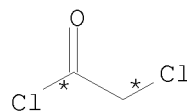
A



BY



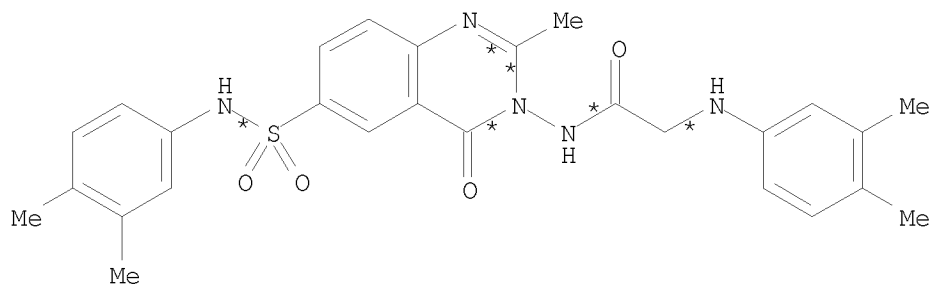
BY



DP

4  
STEPS  
→

10/ 562,112



GM  
YIELD 53%

RX(37) RCT A 181478-44-4, BY 95-64-7

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BZ 774217-21-9

RX(74) RCT BZ 774217-21-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DN 774217-58-2

NTE chemoselective

RX(111) RCT DN 774217-58-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EZ 774217-96-8

RX(149) RCT BY 95-64-7, EZ 774217-96-8



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STAGE(1)

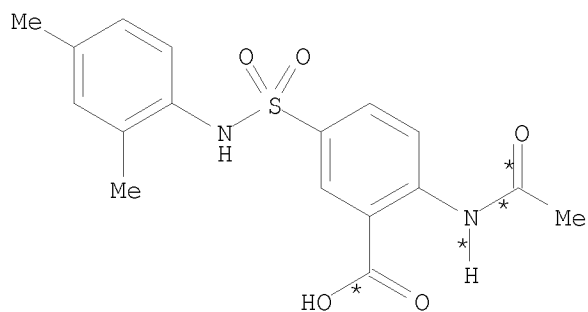
RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

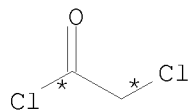
RGT D 7732-18-5 Water  
CON cooled

PRO GM 774218-30-3

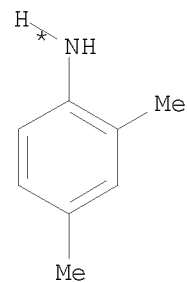
RX(371) OF 372 COMPOSED OF RX(75), RX(112), RX(150)  
RX(371) CB + DP + CA ==> GN



CB

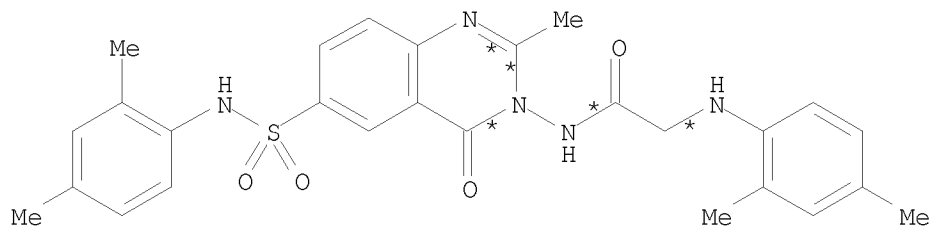


DP



CA

3  
STEPS  
→



GN  
YIELD 65%

RX(75) RCT CB 774217-22-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH

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CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DO 774217-59-3  
NTE chemoselective

RX(112) RCT DO 774217-59-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO FA 774217-97-9

RX(150) RCT CA 95-68-1, FA 774217-97-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

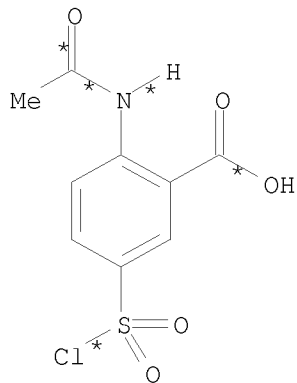
STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

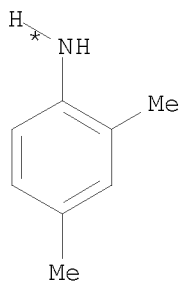
PRO GN 774218-31-4

RX(372) OF 372 COMPOSED OF RX(38), RX(75), RX(112), RX(150)

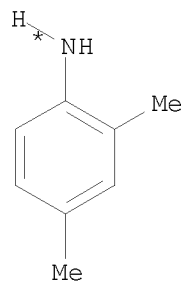
RX(372) A + 2 CA + DP ==> GN



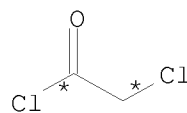
A



CA

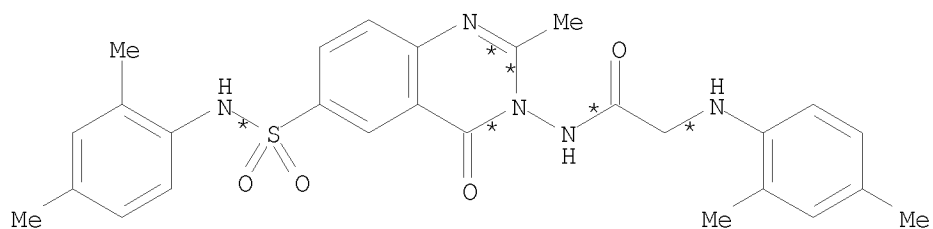


CA



DP

4  
STEPS  
→



GN  
YIELD 65%

RX(38) RCT A 181478-44-4, CA 95-68-1

STAGE(1)

CAT 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO CB 774217-22-0

RX(75) RCT CB 774217-22-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O  
SOL 67-56-1 MeOH  
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water  
CON cooled

PRO DO 774217-59-3  
NTE chemoselective

RX(112) RCT DO 774217-59-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 120 deg C  
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

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CON cooled

PRO FA 774217-97-9

RX(150) RCT CA 95-68-1, FA 774217-97-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO GN 774218-31-4

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 67 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 141:325173 CASREACT

TITLE: Quinazolinone fungal efflux pump inhibitors. Part 2:

In vitro structure-activity relationships of

(N-methylpiperazinyl)-containing derivatives

AUTHOR(S): Watkins, William J.; Lemoine, Remy C.; Chong, Lee;

Cho, Aesop; Renau, Thomas E.; Kuo, Bonnie; Wong,

Vickie; Ludwikow, Maria; Garizi, Negar; Iqbal, Nadeem;

Barnard, John; Jankowska, Renata; Singh, Rajeshwar;

Madsen, Deidre; Lolans, Karen; Lomovskaya, Olga; Oza,

Uma; Dudley, Michael N.

CORPORATE SOURCE: Essential Therapeutics, Inc., Mountain View, CA,

94043, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004),

14(20), 5133-5137

CODEN: BMCLE8; ISSN: 0960-894X

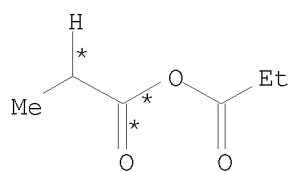
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

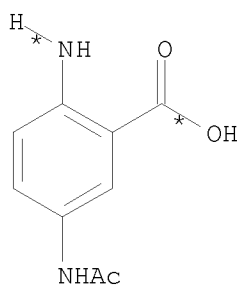
LANGUAGE: English

AB Structure-activity relationships of a novel series of fungal efflux pump inhibitors with respect to potentiation of the activity of fluconazole against strains of *Candida albicans* and *Candida glabrata* over-expressing ABC-type efflux pumps are systematically explored.

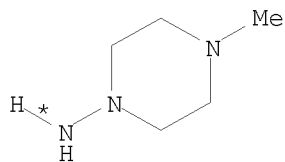
RX(45) OF 108 A + CR + C + F + X ==> CS



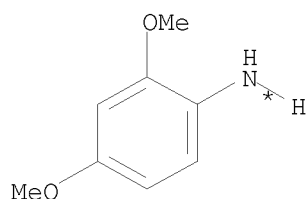
A



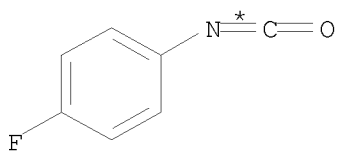
CR



C

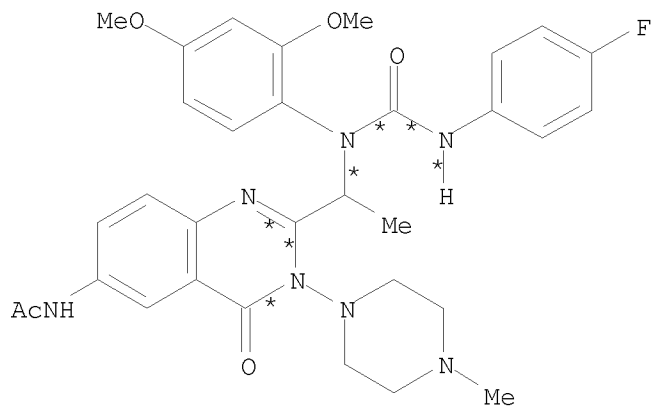


F



X

(45)



CS

RX(45) RCT A 123-62-6, CR 50670-83-2

STAGE(1)

CON 70 deg C

STAGE(2)

RCT C 6928-85-4

SOL 64-19-7 AcOH

CON 70 deg C

STAGE(3)

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RGT H 127-09-3 AcONa, I 7726-95-6 Br2  
SOL 64-19-7 AcOH

STAGE(4)

RCT F 2735-04-8  
SOL 872-50-4 NMEP  
CON 80 deg C

STAGE(5)

RCT X 1195-45-5  
SOL 107-06-2 ClCH2CH2Cl

PRO CS 770746-69-5

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 68 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 141:325172 CASREACT

TITLE: Quinazolinone-based fungal efflux pump inhibitors.  
Part 1: Discovery of an

(N-methylpiperazine)-containing derivative with  
activity in clinically relevant Candida spp.  
AUTHOR(S): Lemoine, Remy C.; Glinka, Tomasz W.; Watkins, William  
J.; Cho, Aesop; Yang, Jessie; Iqbal, Nadeem; Singh,  
Rajeshwar; Madsen, Deidre; Lolans, Karen; Lomovskaya,  
Olga; Oza, Uma; Dudley, Michael N.

CORPORATE SOURCE: Essential Therapeutics, Inc., Mountain View, CA,  
94043, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004),  
14(20), 5127-5131

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

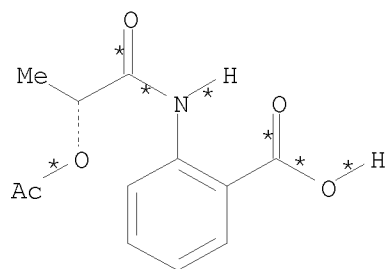
DOCUMENT TYPE: Journal

LANGUAGE: English

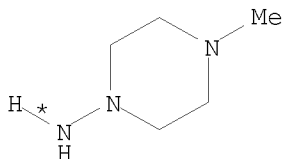
AB The discovery of a series of quinazolinone-based fungal efflux pump  
inhibitors by high-throughput screening for potentiation of fluconazole in  
C. albicans is described. Attempts to improve the aqueous solubility of  
screening  
hits led to the discovery of an analog with greatly improved phys.  
properties and activity against clin.-relevant Candida spp.

RX(17) OF 81 ...AJ + I ==> AM...

10/ 562,112

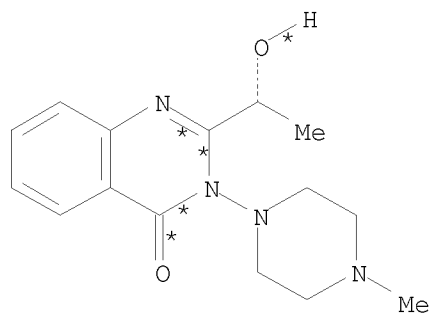


AJ



I

(17)  $\longrightarrow$



AM

RX(17) RCT AJ 770743-64-1

STAGE(1)

RGT AA 108-24-7 Ac2O

CON 70 deg C

STAGE(2)

RCT I 6928-85-4

SOL 64-19-7 AcOH

CON 70 deg C

STAGE(3)

RGT AN 121-44-8 Et3N

SOL 7732-18-5 Water, 67-56-1 MeOH

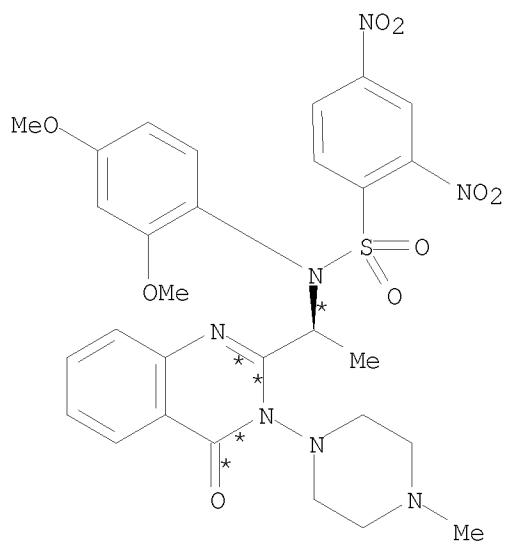
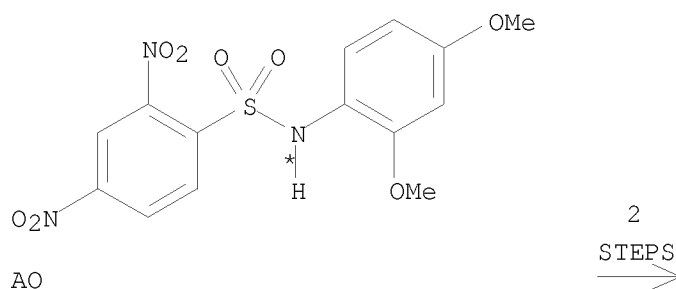
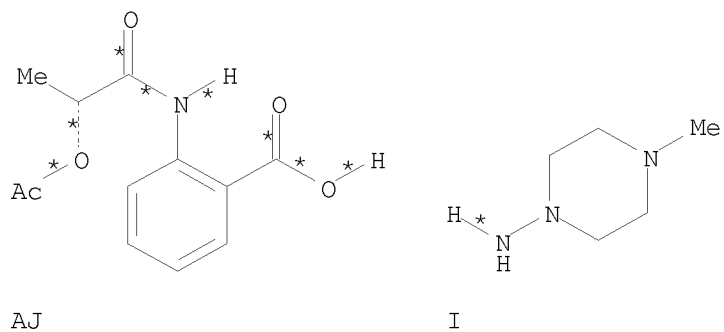
CON room temperature

PRO AM 633305-72-3

RX(41) OF 81 COMPOSED OF RX(17), RX(18)

RX(41) AJ + I + AO ==> AP

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RX(17) RCT AJ 770743-64-1

STAGE(1)

RGT AA 108-24-7 Ac2O  
CON 70 deg C



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STAGE(2)

RCT I 6928-85-4  
SOL 64-19-7 AcOH  
CON 70 deg C

STAGE(3)

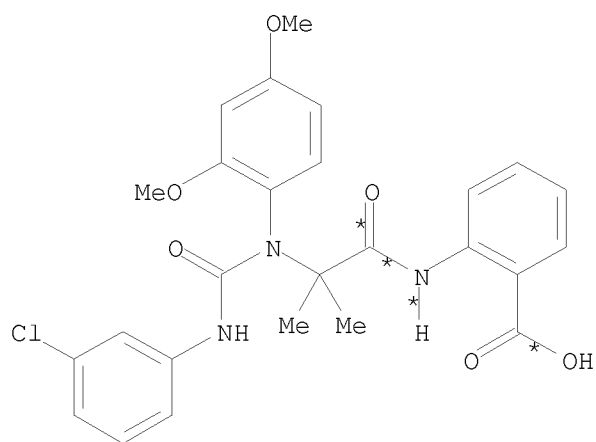
RGT AN 121-44-8 Et3N  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

PRO AM 633305-72-3

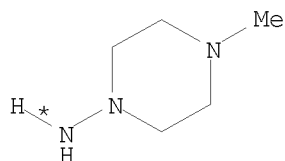
RX(18) RCT AM 633305-72-3, AO 633305-73-4  
RGT AQ 603-35-0 PPh3, AR 2446-83-5 N2(CO2CHMe2)2  
PRO AP 633305-74-5  
SOL 109-99-9 THF  
CON room temperature  
NTE Mitsunobu reaction

RX(47) OF 81 COMPOSED OF RX(25), RX(26)

RX(47) BD + I ==> BF

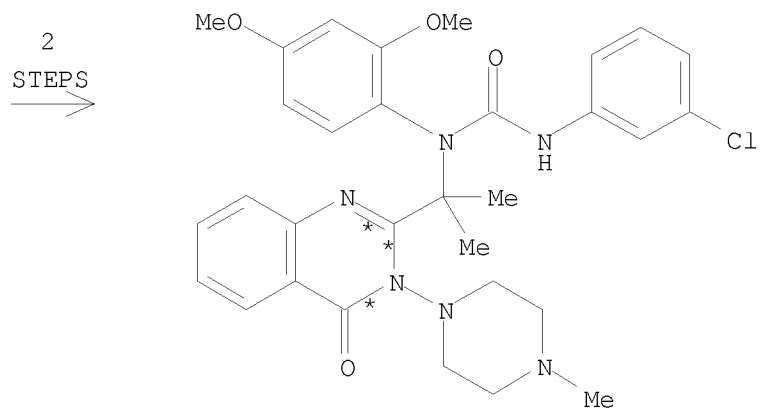


BD



I

10/ 562,112

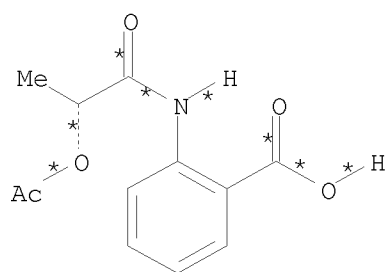


BF

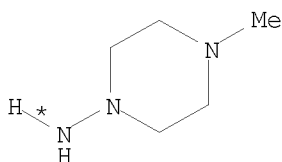
RX(25) RCT BD 770743-67-4  
PRO BE 770743-68-5  
SOL 108-24-7 Ac2O  
CON 80 deg C

RX(26) RCT I 6928-85-4, BE 770743-68-5  
PRO BF 770743-58-3  
SOL 64-19-7 AcOH  
CON 70 deg C

RX(66) OF 81 COMPOSED OF RX(17), RX(18), RX(19)  
RX(66) AJ + I + AO ==> AT

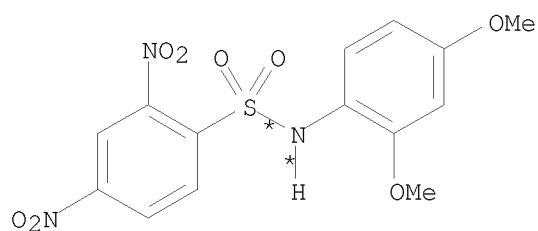


AJ



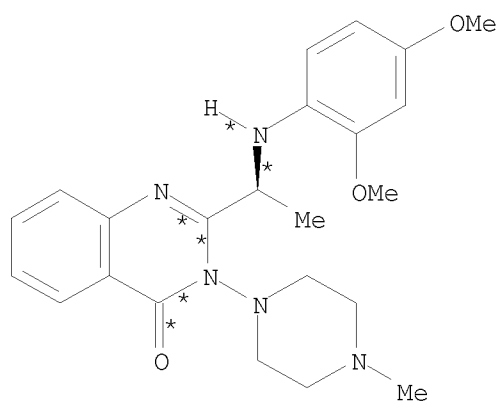
I

10/ 562,112



AO

3  
STEPS  
→



AT

RX(17) RCT AJ 770743-64-1

STAGE(1)

RGT AA 108-24-7 Ac<sub>2</sub>O  
CON 70 deg C

STAGE(2)

RCT I 6928-85-4  
SOL 64-19-7 AcOH  
CON 70 deg C

STAGE(3)

RGT AN 121-44-8 Et<sub>3</sub>N  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON room temperature

PRO AM 633305-72-3

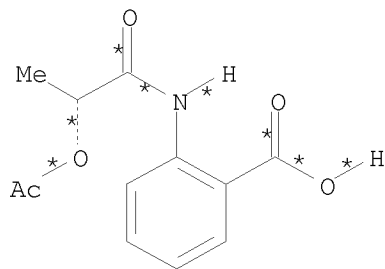
RX(18) RCT AM 633305-72-3, AO 633305-73-4  
RGT AQ 603-35-0 PPh<sub>3</sub>, AR 2446-83-5 N<sub>2</sub>(CO<sub>2</sub>CHMe<sub>2</sub>)<sub>2</sub>  
PRO AP 633305-74-5  
SOL 109-99-9 THF  
CON room temperature  
NTE Mitsunobu reaction

RX(19) RCT AP 633305-74-5

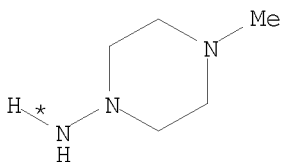
10/ 562,112

RGT AU 68-11-1 HSCH<sub>2</sub>CO<sub>2</sub>H, AN 121-44-8 Et<sub>3</sub>N  
PRO AT 633305-75-6  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON room temperature

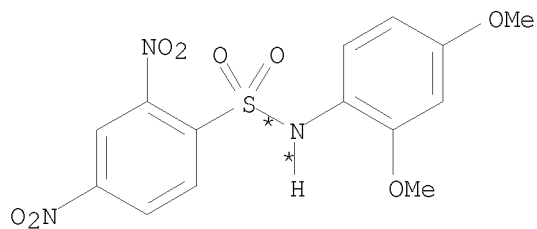
RX(69) OF 81 COMPOSED OF RX(17), RX(18), RX(19), RX(20)  
RX(69) AJ + I + AO + V ==> AV



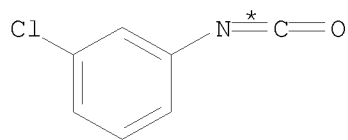
AJ



I



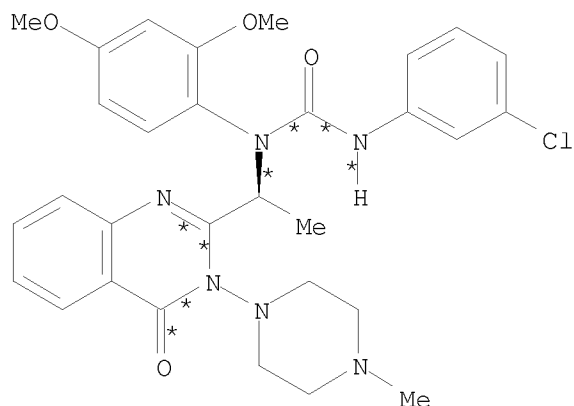
AO



V

4  
STEPS  
→

10/ 562,112



AV

RX(17) RCT AJ 770743-64-1

STAGE(1)

RGT AA 108-24-7 Ac2O

CON 70 deg C

STAGE(2)

RCT I 6928-85-4

SOL 64-19-7 AcOH

CON 70 deg C

STAGE(3)

RGT AN 121-44-8 Et3N

SOL 7732-18-5 Water, 67-56-1 MeOH

CON room temperature

PRO AM 633305-72-3

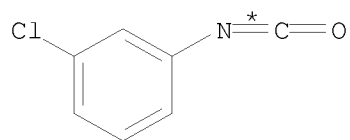
RX(18) RCT AM 633305-72-3, AO 633305-73-4  
RGT AQ 603-35-0 PPh3, AR 2446-83-5 N2(CO2CHMe2)2  
PRO AP 633305-74-5  
SOL 109-99-9 THF  
CON room temperature  
NTE Mitsunobu reaction

RX(19) RCT AP 633305-74-5  
RGT AU 68-11-1 HSCH2CO2H, AN 121-44-8 Et3N  
PRO AT 633305-75-6  
SOL 75-09-2 CH2Cl2  
CON room temperature

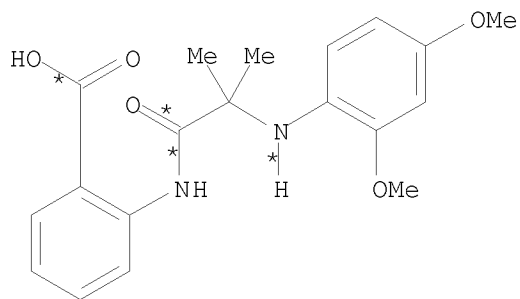
RX(20) RCT AT 633305-75-6, V 2909-38-8  
PRO AV 770743-59-4  
SOL 75-09-2 CH2Cl2  
CON room temperature

RX(73) OF 81 COMPOSED OF RX(24), RX(25), RX(26)  
RX(73) V + BA + I ==> BF

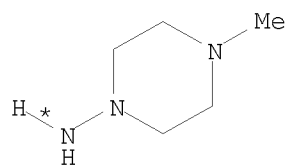
10/ 562,112



V

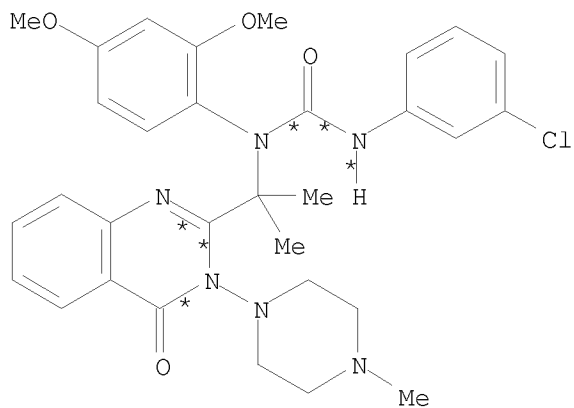


BA



I

3  
STEPS  
→



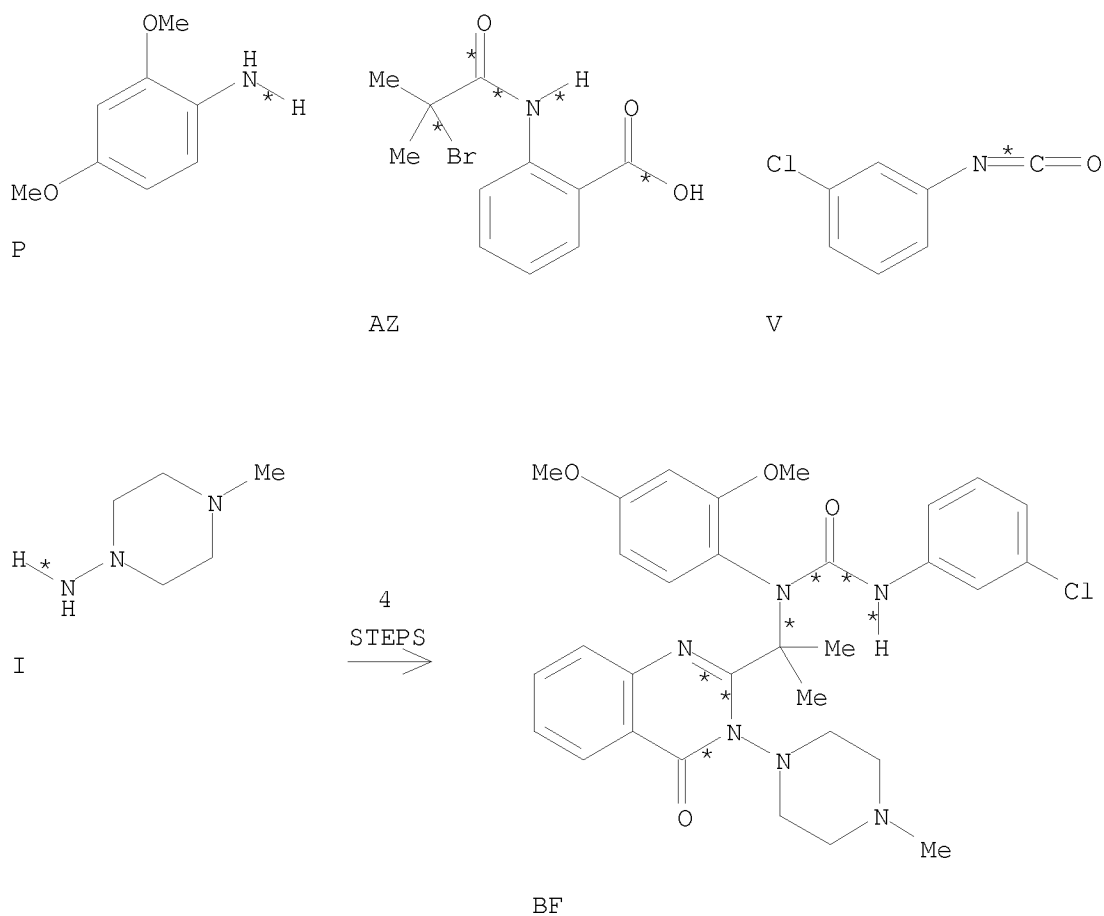
BF

RX(24) RCT V 2909-38-8, BA 770743-66-3  
PRO BD 770743-67-4  
SOL 75-09-2 CH2Cl2  
CON room temperature

RX(25) RCT BD 770743-67-4  
PRO BE 770743-68-5  
SOL 108-24-7 Ac2O  
CON 80 deg C

RX(26) RCT I 6928-85-4, BE 770743-68-5  
PRO BF 770743-58-3  
SOL 64-19-7 AcOH  
CON 70 deg C

RX(74) OF 81 COMPOSED OF RX(23), RX(24), RX(25), RX(26)  
RX(74) P + AZ + V + I ==> BF



RX(23) RCT P 2735-04-8, AZ 770743-65-2  
 RGT BB 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO BA 770743-66-3  
 SOL 64-17-5 EtOH  
 CON reflux

RX(24) RCT V 2909-38-8, BA 770743-66-3  
 PRO BD 770743-67-4  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON room temperature

RX(25) RCT BD 770743-67-4  
 PRO BE 770743-68-5  
 SOL 108-24-7 Ac<sub>2</sub>O  
 CON 80 deg C

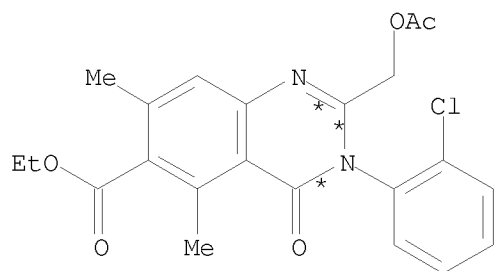
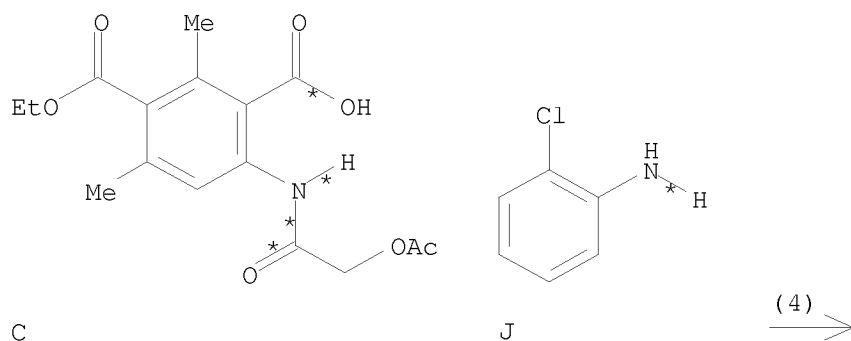
RX(26) RCT I 6928-85-4, BE 770743-68-5  
 PRO BF 770743-58-3  
 SOL 64-19-7 AcOH  
 CON 70 deg C

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 69 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 141:314290 CASREACT  
 TITLE: A Facile Synthesis of  
 C2,N3-Disubstituted-4-quinazolone  
 AUTHOR(S): Xue, Song; McKenna, Joseph; Shieh, Wen-Chung; Repic,  
 Oljan  
 CORPORATE SOURCE: Chemical and Analytical Development, Novartis  
 Institute for Biomedical Research, East Hanover, NJ,  
 07936, USA  
 SOURCE: Journal of Organic Chemistry (2004), 69(19), 6474-6477  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A simple and efficient methodol. for the synthesis of C2,N3-disubstituted  
 4-quinazolones from anilines and N-acetylanthranilic acids was developed.  
 The new cyclization conditions are much milder than any other reported  
 protocols and resulted in excellent yields (87-98%) without chromatog.

RX(4) OF 49 ...C + J ==> K...



K  
 YIELD 95%

RX(4) RCT C 768368-41-8, J 95-51-2

STAGE(1)



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RGT L 7719-12-2 PC13  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 50 deg C  
SUBSTAGE(3) 2 hours, 50 deg C  
SUBSTAGE(4) 50 deg C -> room temperature

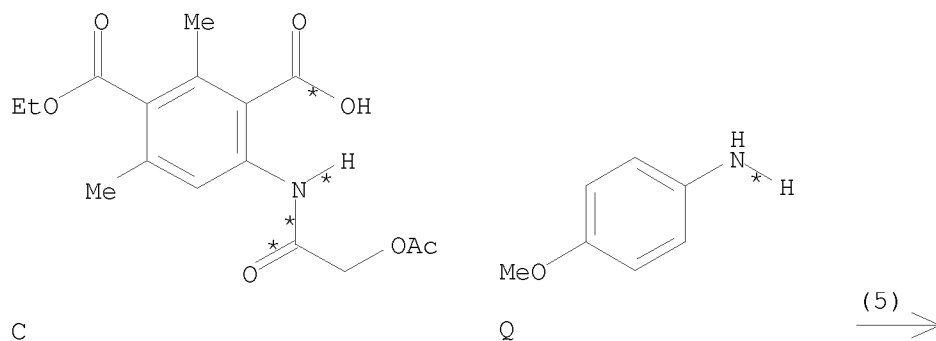
STAGE(2)

RGT M 7647-01-0 HCl  
SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO K 768368-42-9

NTE optimization study, optimized on solvent

RX(5) OF 49 ...C + Q ==> R...



R  
YIELD 94%

RX(5) RCT C 768368-41-8, Q 104-94-9

STAGE(1)

RGT L 7719-12-2 PC13  
SOL 75-05-8 MeCN  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature -> 50 deg C  
SUBSTAGE(3) 2 hours, 50 deg C  
SUBSTAGE(4) 50 deg C -> room temperature

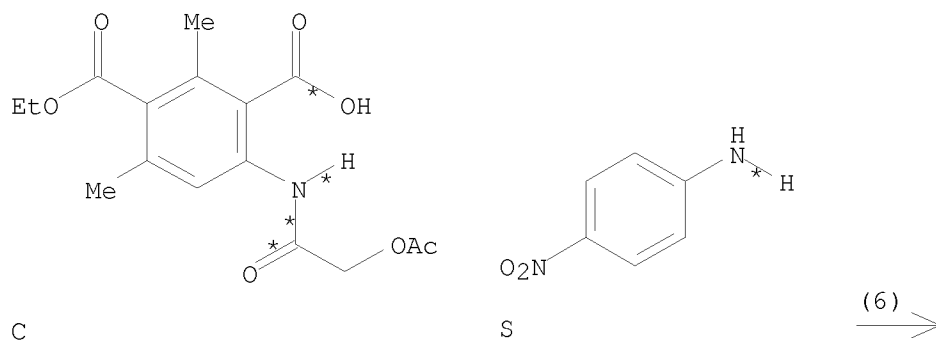
STAGE(2)

RGT M 7647-01-0 HCl  
SOL 141-78-6 AcOEt, 7732-18-5 Water

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PRO R 768368-43-0

RX(6) OF 49 ...C + S ==> T...



T  
YIELD 96%

RX(6) RCT C 768368-41-8, S 100-01-6

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

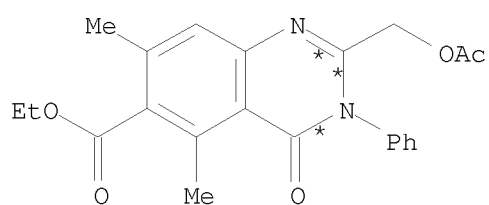
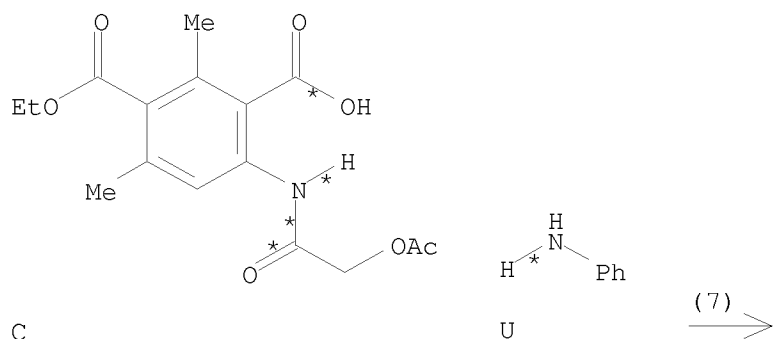
RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO T 768368-44-1

RX(7) OF 49 ...C + U ==> V...

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V  
YIELD 93%

RX(7) RCT C 768368-41-8, U 62-53-3

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

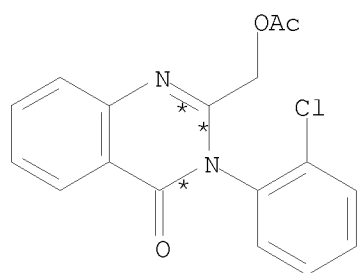
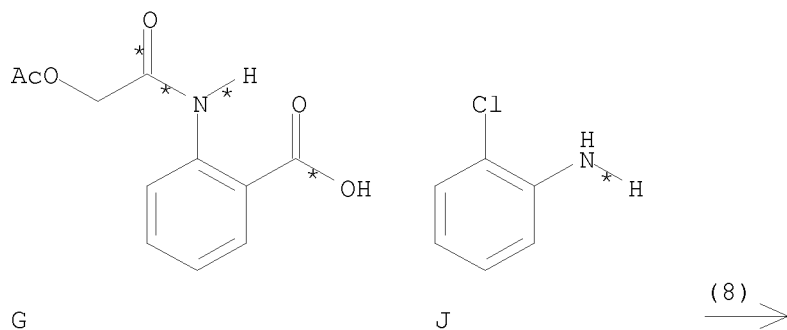
RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO V 77307-63-2

RX(8) OF 49 ...G + J ==> W...

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W  
YIELD 96%

RX(8) RCT G 51815-70-4, J 95-51-2

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

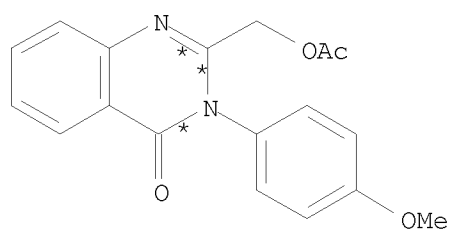
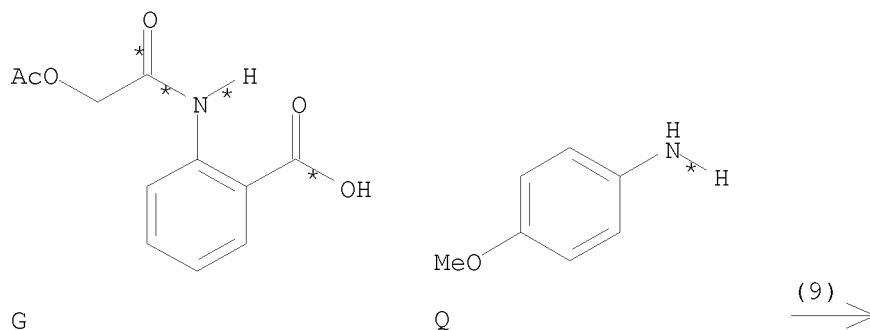
RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO W 54995-77-6

RX(9) OF 49 ...G + Q ==> X...

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X  
YIELD 97%

RX(9) RCT G 51815-70-4, Q 104-94-9

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

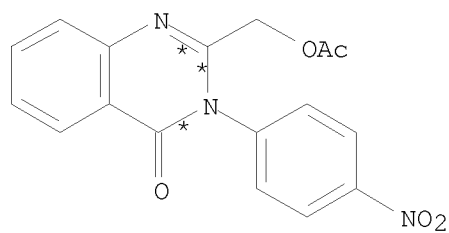
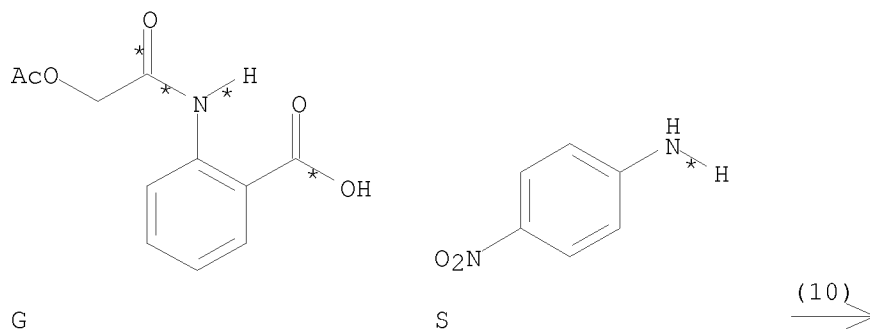
RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO X 768368-45-2

RX(10) OF 49 ...G + S ==> Y...

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Y  
YIELD 98%

RX(10) RCT G 51815-70-4, S 100-01-6

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

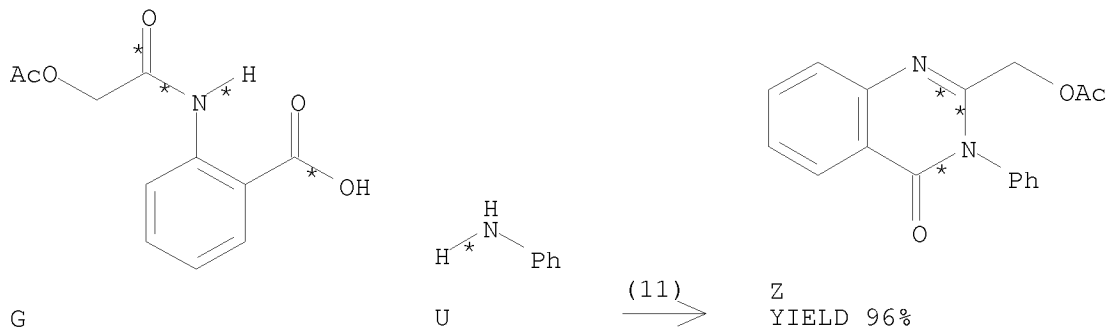
RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO Y 768368-46-3

RX(11) OF 49 ...G + U ==> Z...

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RX(11) RCT G 51815-70-4, U 62-53-3

STAGE (1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE (3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

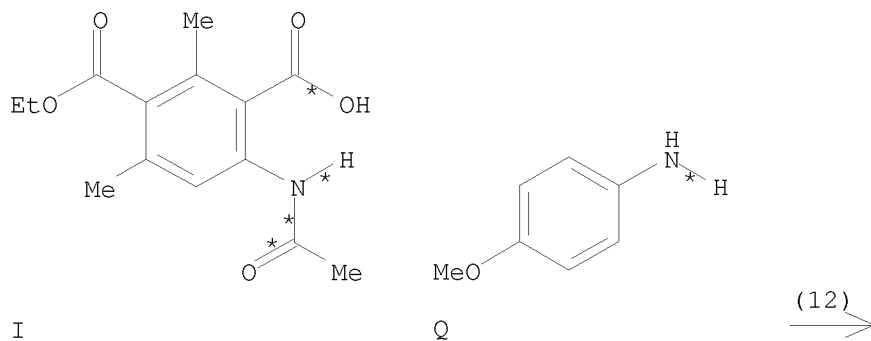
STAGE (2)

RGT M 7647-01-0 HCL

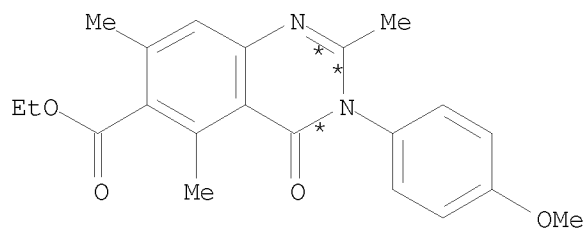
SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO Z 20873-19-2

RX(12) OF 49      ...I   +   Q   ==>   AA



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AA

YIELD 90%

RX(12) RCT I 75958-37-1, Q 104-94-9

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 20 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

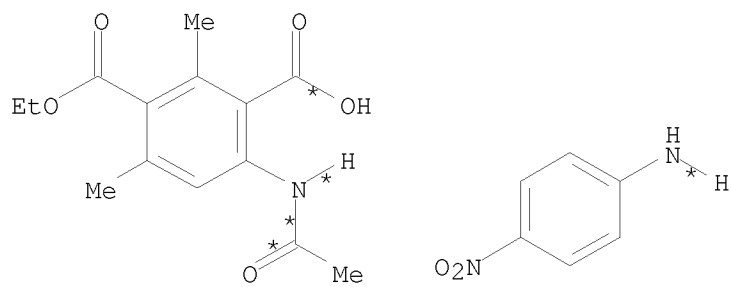
STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO AA 768368-47-4

RX(13) OF 49 ...I + S ==> AB



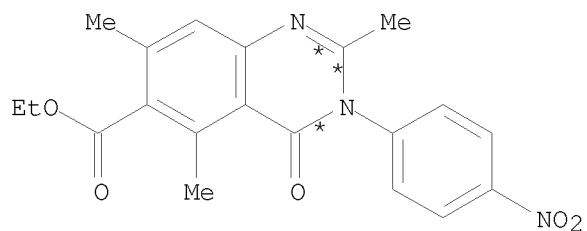
I

S

(13)  
→



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AB  
YIELD 96%

RX(13) RCT I 75958-37-1, S 100-01-6

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

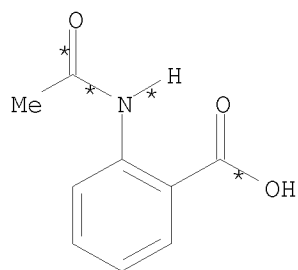
STAGE(2)

RGT M 7647-01-0 HCl

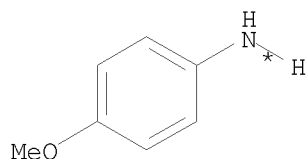
SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO AB 768368-48-5

RX(14) OF 49 AC + Q ==> AD



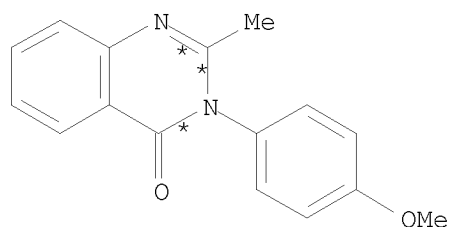
AC



Q

(14)  
→

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AD  
YIELD 87%

RX(14) RCT AC 89-52-1, Q 104-94-9

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 20 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

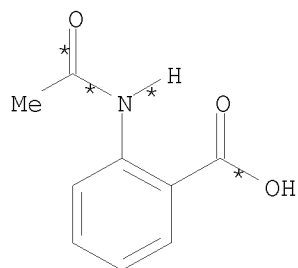
STAGE(2)

RGT M 7647-01-0 HCl

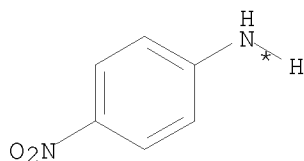
SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO AD 30507-16-5

RX(15) OF 49 AC + S ==> AE



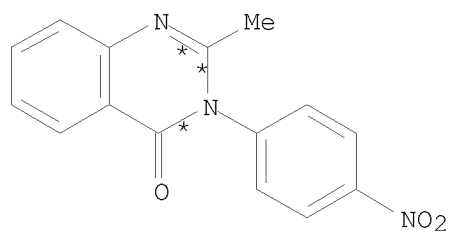
AC



S

(15)  $\longrightarrow$

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AE  
YIELD 89%

RX(15) RCT AC 89-52-1, S 100-01-6

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 20 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

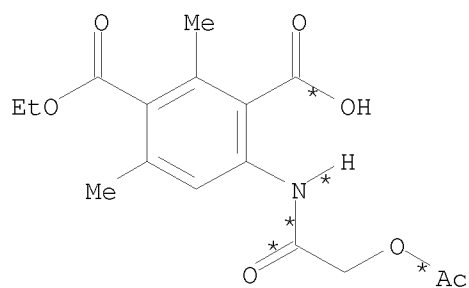
RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

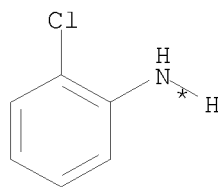
PRO AE 1788-96-1

RX(34) OF 49 COMPOSED OF RX(4), RX(16)

RX(34) C + J ==> AF



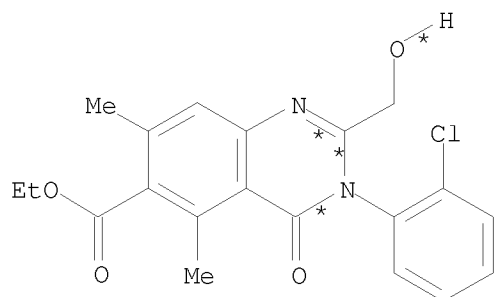
C



J

2  
STEPS  
=>

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AF  
YIELD 95%

RX(4) RCT C 768368-41-8, J 95-51-2

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO K 768368-42-9

NTE optimization study, optimized on solvent

RX(16)

RCT K 768368-42-9

RGT AG 584-08-7 K<sub>2</sub>CO<sub>3</sub>

PRO AF 75913-83-6

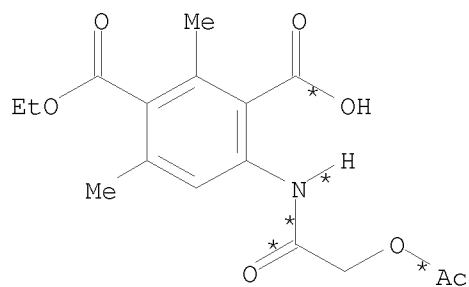
SOL 67-56-1 MeOH

CON SUBSTAGE(1) room temperature

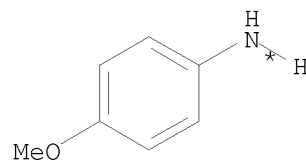
SUBSTAGE(2) 20 minutes, room temperature

RX(35) OF 49 COMPOSED OF RX(5), RX(17)

RX(35) C + Q ==> AI



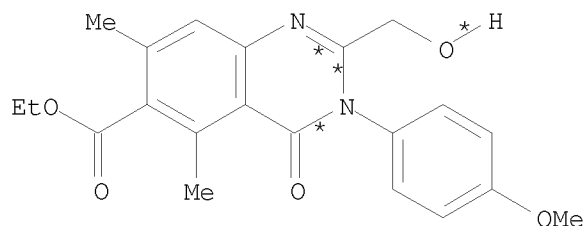
C



Q

2  
STEPS  
→

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● HCl

AI  
YIELD 90%

RX(5) RCT C 768368-41-8, Q 104-94-9

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO R 768368-43-0

RX(17) RCT R 768368-43-0

STAGE(1)

RGT AG 584-08-7 K2CO3

SOL 67-56-1 MeOH

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 20 minutes, room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 7732-18-5 Water

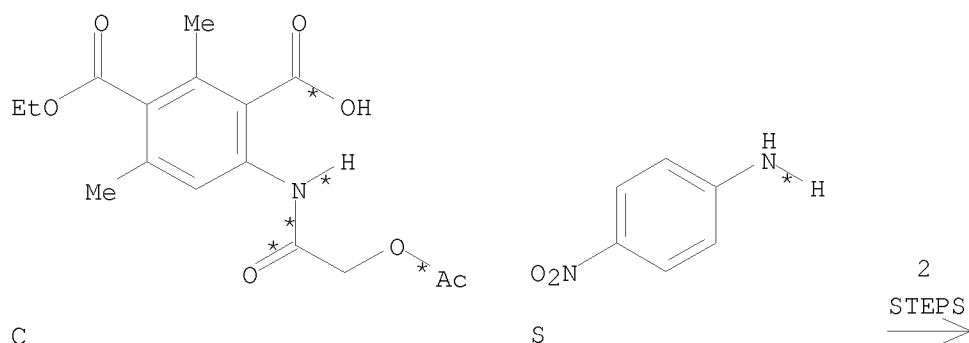
CON room temperature

PRO AI 768368-49-6

RX(36) OF 49 COMPOSED OF RX(6), RX(18)

RX(36) C + S ==> AJ

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AJ  
YIELD 95%

RX(6) RCT C 768368-41-8, S 100-01-6

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO T 768368-44-1

RX(18)

RCT T 768368-44-1

RGT AG 584-08-7 K2CO3

PRO AJ 768368-50-9

SOL 67-56-1 MeOH

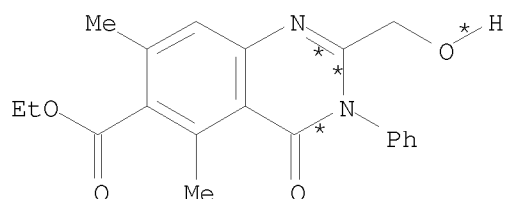
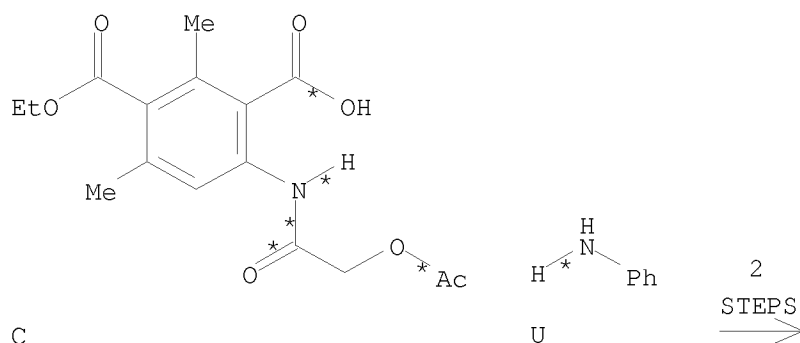
CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 20 minutes, room temperature

RX(37) OF 49 COMPOSED OF RX(7), RX(19)

RX(37) C + U ==> AK

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AK  
YIELD 96%

RX(7) RCT C 768368-41-8, U 62-53-3

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO V 77307-63-2

RX(19) RCT V 77307-63-2

RGT AG 584-08-7 K2CO3

PRO AK 77307-64-3

SOL 67-56-1 MeOH

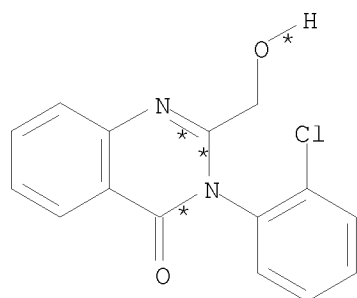
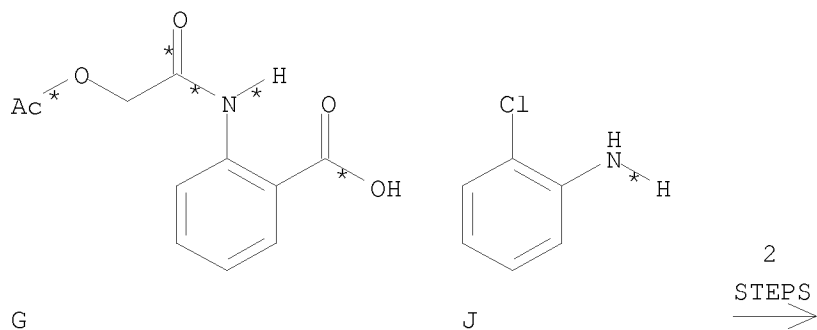
CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 20 minutes, room temperature

RX(38) OF 49 COMPOSED OF RX(8), RX(20)

RX(38) G + J ==> AL

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AL  
YIELD 95%

RX(8) RCT G 51815-70-4, J 95-51-2

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO W 54995-77-6

RX(20)

RCT W 54995-77-6

RGT AG 584-08-7 K<sub>2</sub>CO<sub>3</sub>

PRO AL 29909-21-5

SOL 67-56-1 MeOH

CON SUBSTAGE(1) room temperature

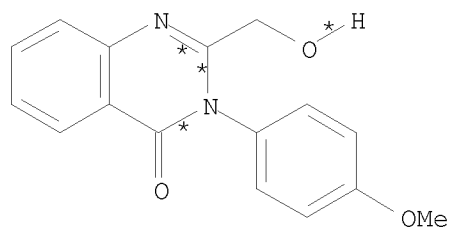
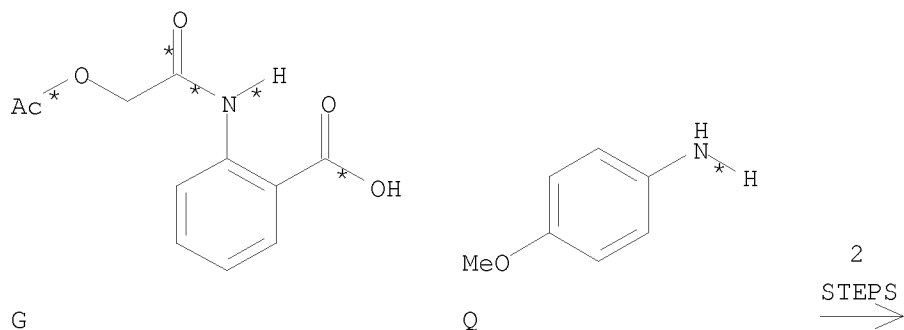
SUBSTAGE(2) 20 minutes, room temperature

RX(39) OF 49 COMPOSED OF RX(9), RX(21)

RX(39) G + Q ==> AM



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AM  
YIELD 90%

RX(9) RCT G 51815-70-4, Q 104-94-9

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO X 768368-45-2

RX(21)

RCT X 768368-45-2

RGT AG 584-08-7 K2CO3

PRO AM 53615-54-6

SOL 67-56-1 MeOH

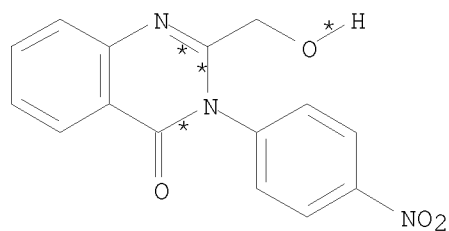
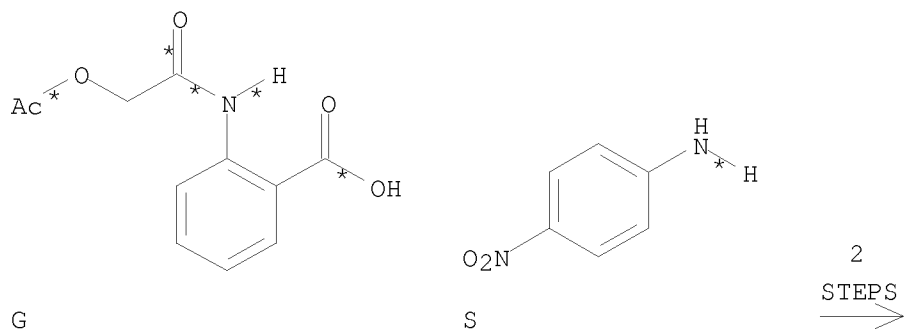
CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 20 minutes, room temperature

RX(40) OF 49 COMPOSED OF RX(10), RX(22)

RX(40) G + S ==> AN

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AN  
YIELD 91%

RX(10) RCT G 51815-70-4, S 100-01-6

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO Y 768368-46-3

RX(22)

RCT Y 768368-46-3

RGT AG 584-08-7 K2CO3

PRO AN 768368-51-0

SOL 67-56-1 MeOH

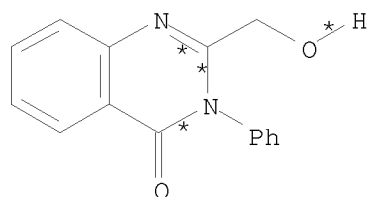
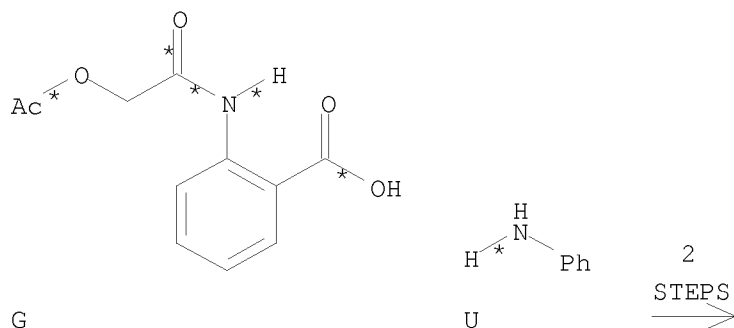
CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 20 minutes, room temperature

RX(41) OF 49 COMPOSED OF RX(11), RX(23)

RX(41) G + U ==> AO

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AO  
YIELD 91%

RX(11) RCT G 51815-70-4, U 62-53-3

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO Z 20873-19-2

RX(23)

RCT Z 20873-19-2

RGT AG 584-08-7 K<sub>2</sub>CO<sub>3</sub>

PRO AO 20873-20-5

SOL 67-56-1 MeOH

CON SUBSTAGE(1) room temperature

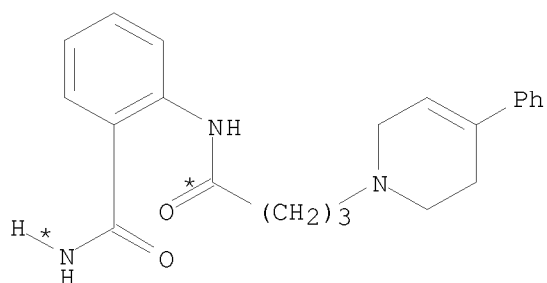
SUBSTAGE(2) 20 minutes, room temperature

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

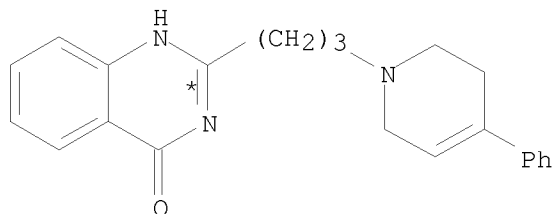
ACCESSION NUMBER: 141:288542 CASREACT  
 TITLE: Rational Approaches to Discovery of Orally Active and Brain-Penetrable Quinazolinone Inhibitors of Poly(ADP-ribose)polymerase  
 AUTHOR(S): Hattori, Kouji; Kido, Yoshiyuki; Yamamoto, Hirofumi; Ishida, Junya; Kamijo, Kazunori; Murano, Kenji; Ohkubo, Mitsuru; Kinoshita, Takayoshi; Iwashita, Akinori; Mihara, Kayoko; Yamazaki, Syunji; Matsuoka, Nobuya; Teramura, Yoshinori; Miyake, Hiroshi  
 CORPORATE SOURCE: Medicinal Chemistry Research Laboratories, Exploratory Research Laboratories, Medicinal Biology Research Laboratories, and Biopharmaceutical and Pharmacokinetic Research Laboratories, Fujisawa Pharmaceutical Co., Ltd., Osaka, 532-8514, Japan  
 SOURCE: Journal of Medicinal Chemistry (2004), 47(17), 4151-4154  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A novel class of quinazolinone derivs. as potent poly(ADP-ribose)polymerase-1 (PARP-1) inhibitors has been discovered. Key to success was application of a rational discovery strategy involving structure-based design, combinatorial chemical, and classical SAR for improvement of potency and bioavailability. The new inhibitors were shown to bind to the nicotinamide-ribose binding site (NI site) and the adenosine-ribose binding site (AD site) of NAD<sup>+</sup>.

RX(32) OF 35 ...BR ==> D



BR



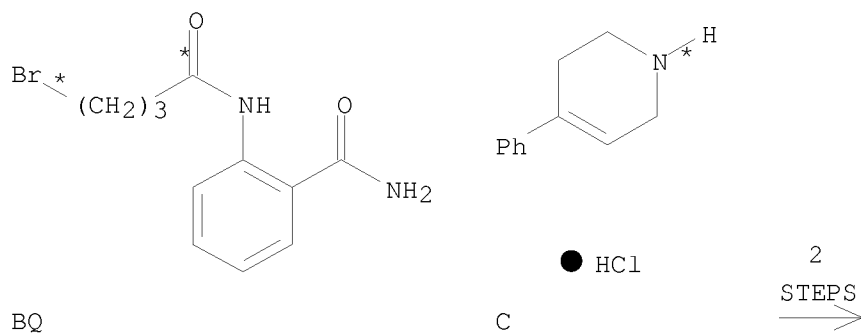
D  
 YIELD 73%

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RX(32)     RCT   BR 437998-41-9  
             RGT   J 1310-73-2 NaOH  
             PRO   D 437995-37-4  
             SOL   7732-18-5 Water, 123-91-1 Dioxane  
             CON   15 hours, room temperature  
             NTE   alternate solid-supported preparation also described, other  
                     analogs similarly prepared

RX(34) OF 35 COMPOSED OF RX(31), RX(32)

RX(34)     BQ   +   C   ==>   D



D  
YIELD 73%

RX(31)     RCT   BQ 437998-35-1, C 43064-12-6

STAGE(1)

RGT   BS 121-44-8 Et3N

SOL   68-12-2 DMF

CON   SUBSTAGE(1) 0 deg C -> room temperature

         SUBSTAGE(2) 24 hours, room temperature

STAGE(2)

RGT   N 7732-18-5 Water

CON   room temperature

PRO   BR 437998-41-9

RX(32)     RCT   BR 437998-41-9  
             RGT   J 1310-73-2 NaOH

PRO D 437995-37-4  
 SOL 7732-18-5 Water, 123-91-1 Dioxane  
 CON 15 hours, room temperature  
 NTE alternate solid-supported preparation also described, other  
 analogs similarly prepared

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 71 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 141:225440 CASREACT

TITLE: Synthesis of some quinazolinone derivatives as  
 possible anticancer agents

AUTHOR(S): Murugan, V.; Padmavathy, N. P.; Ramasarma, G. V. S.;  
 Sharma, Sunil V.; Suresh, B.

CORPORATE SOURCE: Department of Pharmaceutical Chemistry, JSS College of  
 Pharmacy, Ooty, 643 001, India

SOURCE: Indian Journal of Heterocyclic Chemistry (2003),  
 13(2), 143-146

CODEN: IJCHEI; ISSN: 0971-1627

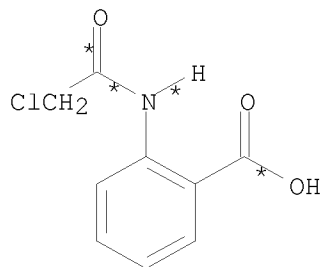
PUBLISHER: Prof. R. S. Varma

DOCUMENT TYPE: Journal

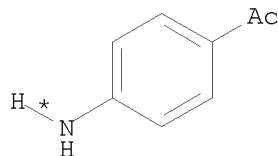
LANGUAGE: English

AB The title compds. 4-Chloro-1-[4-(6,8-disubstituted-2-chloromethyl-  
 quinazolin-4-one-3-yl)-phenyl]butane-1,3-dione derivs. were synthesized by  
 the reaction of corresponding 2-chloromethyl-3-(acetophenon-4-yl)-4-  
 (3H)quinazolinone with Et chloroacetate in diispropylether and NaOMe in  
 dry methanol. Compound 2-(N-morpholinomethyl)-3-(acetophenon-4-yl)-4-(3H)  
 quinazolinone was prepared by the reaction of  
 2-chloromethyl-3-(acetophenon-4-yl)-4-(3H)quinazolinone and morpholine in  
 the presence of potassium carbonate in dry methanol. The intermediates  
 N-chloroacetyl anthranilic acid derivs. and  
 2-chloromethyl-3-(acetophenon-4-yl)-4-(3H) quinazolinones were prepared by  
 standard procedures. All the intermediates and title compds. were  
 characterized by phys., chemical, anal. and spectral data. The biol.  
 evaluation of the compds. was carried out by various methods such as short  
 term study for in-vitro antitumor activity, cytostatic activity and  
 antioxidant activity. Compds. 4-Chloro-1-[4-(6,8-dibromo-, 6,8-dichloro-,  
 and 6-iodo-substituted-2-chloromethyl-quinazolin-4-one-3-yl)-phenyl]butane-  
 1,3-diones showed significant anticancer activity.

RX(1) OF 17 A + B ==> C...



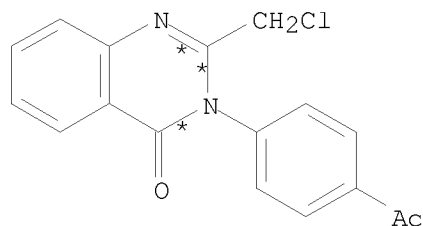
A



B



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C  
YIELD 52%

RX(1) RCT A 14422-49-2, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

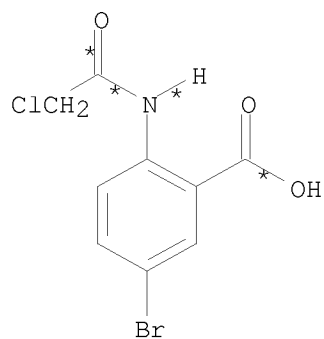
RGT E 144-55-8 NaHCO3

SOL 7732-18-5 Water

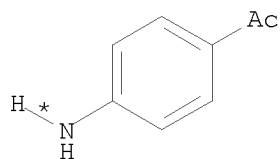
CON neutralized

PRO C 748165-98-2

RX(2) OF 17 H + B ==> I...



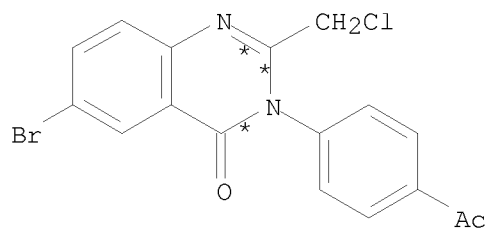
H



B

(2)  $\longrightarrow$

10/ 562,112



I  
YIELD 69%

RX(2) RCT H 155104-20-4, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

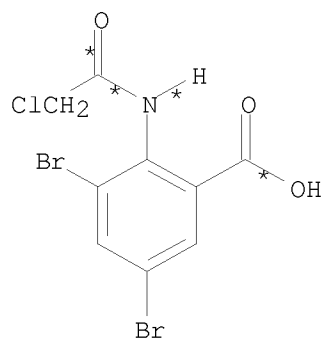
RGT E 144-55-8 NaHCO3

SOL 7732-18-5 Water

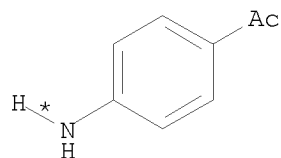
CON neutralized

PRO I 748165-99-3

RX(3) OF 17 J + B ==> K...



J

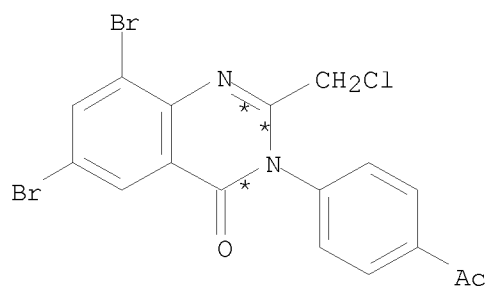


B

(3) >



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K  
YIELD 51%

RX(3) RCT J 103952-88-1, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

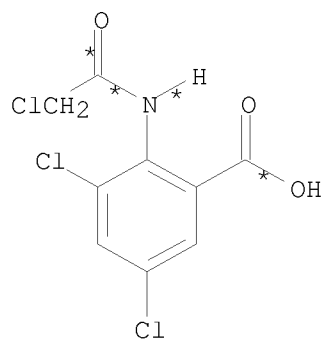
RGT E 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water

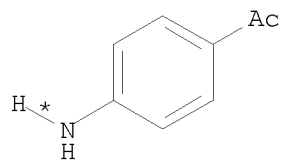
CON neutralized

PRO K 748166-00-9

RX(4) OF 17 L + B ==> M...



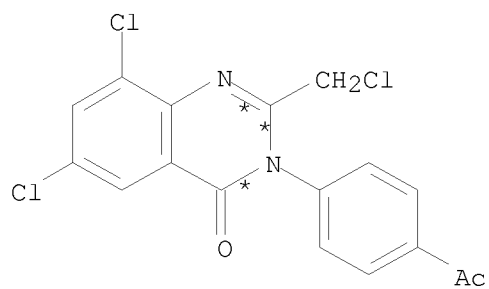
L



B

(4)  $\longrightarrow$

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M  
YIELD 66%

RX(4) RCT L 39263-98-4, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

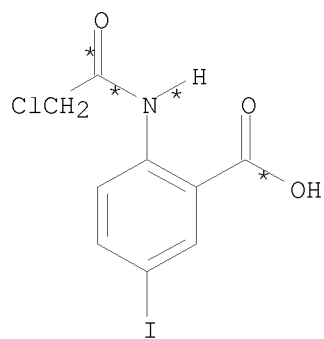
RGT E 144-55-8 NaHCO3

SOL 7732-18-5 Water

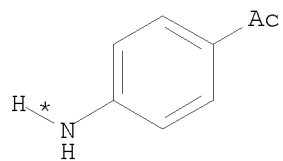
CON neutralized

PRO M 748166-01-0

RX(5) OF 17 N + B ==> O...



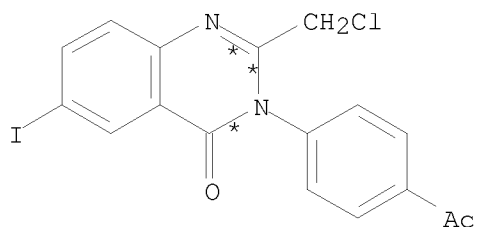
N



B

(5)  $\longrightarrow$

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O  
YIELD 71%

RX(5) RCT N 175850-45-0, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT E 144-55-8 NaHCO<sub>3</sub>

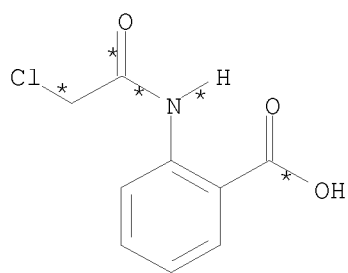
SOL 7732-18-5 Water

CON neutralized

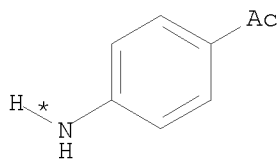
PRO O 748166-02-1

RX(12) OF 17 COMPOSED OF RX(1), RX(6)

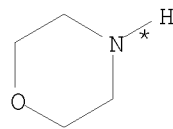
RX(12) A + B + P ==> Q



A



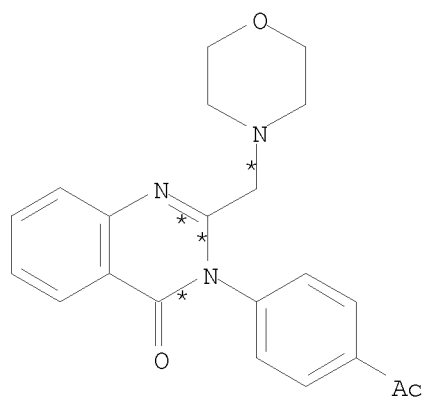
B



P

2  
STEPS  
→

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Q  
YIELD 70%

RX(1) RCT A 14422-49-2, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13  
SOL 108-88-3 PhMe  
CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT E 144-55-8 NaHCO3  
SOL 7732-18-5 Water  
CON neutralized

PRO C 748165-98-2

RX(6) RCT C 748165-98-2, P 110-91-8

RGT R 584-08-7 K2CO3

PRO Q 748166-08-7

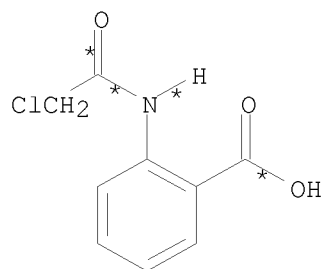
SOL 67-56-1 MeOH

CON 4 hours, reflux

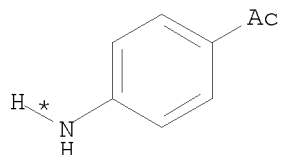
RX(13) OF 17 COMPOSED OF RX(1), RX(11)

RX(13) A + B + T ==> AC

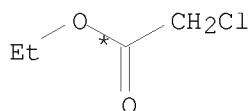
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A

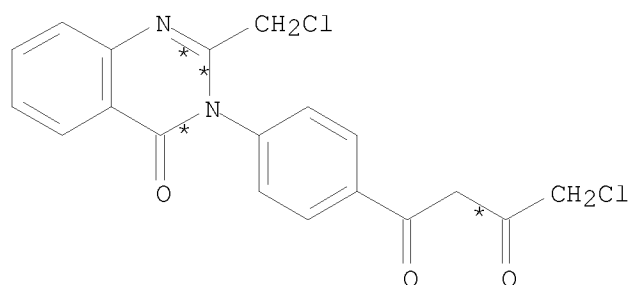


B



T

2  
STEPS  
→



AC  
YIELD 58%

RX(1) RCT A 14422-49-2, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT E 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water

CON neutralized

PRO C 748165-98-2

RX(11) RCT T 105-39-5

STAGE(1)

RGT V 124-41-4 NaOMe

SOL 67-56-1 MeOH, 108-20-3 Isopropyl ether

CON 5 minutes, room temperature

STAGE(2)

RCT C 748165-98-2

SOL 108-20-3 Isopropyl ether

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CON SUBSTAGE(1) 5 minutes, room temperature  
SUBSTAGE(2) 24 hours, reflux

STAGE(3)

RGT W 7647-01-0 HCl  
SOL 7732-18-5 Water

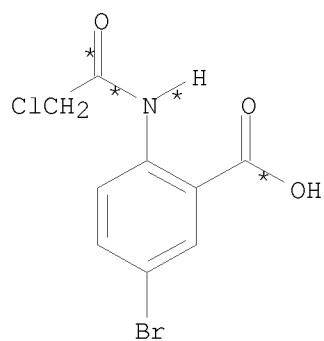
STAGE(4)

RGT X 497-19-8 Na2CO3  
SOL 7732-18-5 Water  
CON neutralized

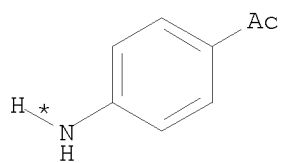
PRO AC 748166-03-2

RX(14) OF 17 COMPOSED OF RX(2), RX(7)

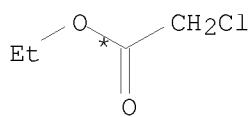
RX(14) H + B + T ==> U



H

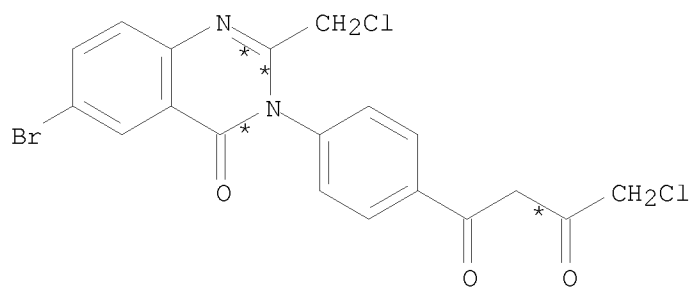


B



T

2  
STEPS  
→



U  
YIELD 67%

RX(2) RCT H 155104-20-4, B 99-92-3

STAGE(1)

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RGT D 7719-12-2 PC13  
SOL 108-88-3 PhMe  
CON 3 hours, reflux

STAGE(2)  
SOL 7732-18-5 Water

STAGE(3)  
RGT E 144-55-8 NaHCO3  
SOL 7732-18-5 Water  
CON neutralized

PRO I 748165-99-3

RX(7) RCT T 105-39-5

STAGE(1)  
RGT V 124-41-4 NaOMe  
SOL 67-56-1 MeOH, 108-20-3 Isopropyl ether  
CON 5 minutes, room temperature

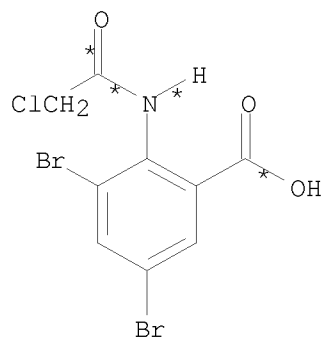
STAGE(2)  
RCT I 748165-99-3  
SOL 108-20-3 Isopropyl ether  
CON SUBSTAGE(1) 5 minutes, room temperature  
SUBSTAGE(2) 24 hours, reflux

STAGE(3)  
RGT W 7647-01-0 HCl  
SOL 7732-18-5 Water

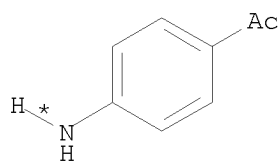
STAGE(4)  
RGT X 497-19-8 Na2CO3  
SOL 7732-18-5 Water  
CON neutralized

PRO U 748166-04-3

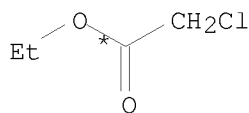
RX(15) OF 17 COMPOSED OF RX(3), RX(8)  
RX(15) J + B + T ==> Z



J



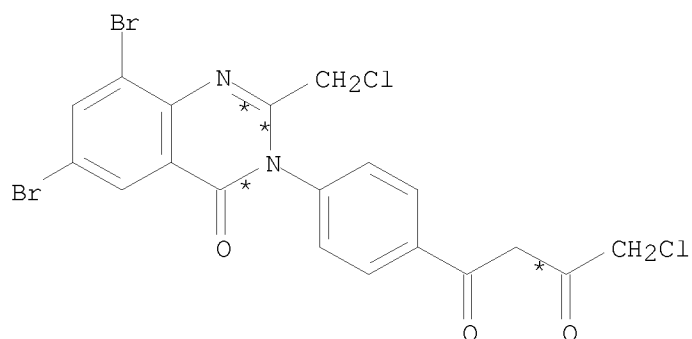
B



T

10/ 562,112

2  
STEPS  
→



Z  
YIELD 52%

RX(3) RCT J 103952-88-1, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT E 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water

CON neutralized

PRO K 748166-00-9

RX(8) RCT T 105-39-5

STAGE(1)

RGT V 124-41-4 NaOMe

SOL 67-56-1 MeOH, 108-20-3 Isopropyl ether

CON 5 minutes, room temperature

STAGE(2)

RCT K 748166-00-9

SOL 108-20-3 Isopropyl ether

CON SUBSTAGE(1) 5 minutes, room temperature

SUBSTAGE(2) 24 hours, reflux

STAGE(3)

RGT W 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(4)

RGT X 497-19-8 Na<sub>2</sub>CO<sub>3</sub>

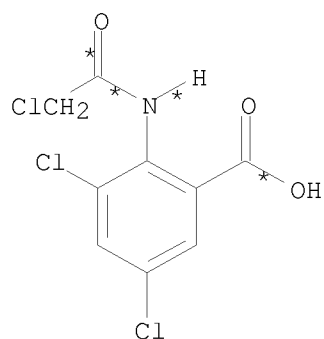


10/ 562,112

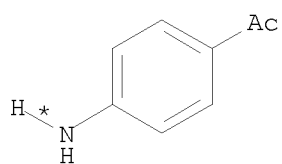
SOL 7732-18-5 Water  
CON neutralized

PRO Z 748166-05-4

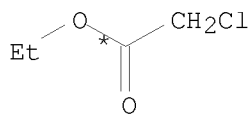
RX(16) OF 17 COMPOSED OF RX(4), RX(9)  
RX(16) L + B + T ==> AA



L

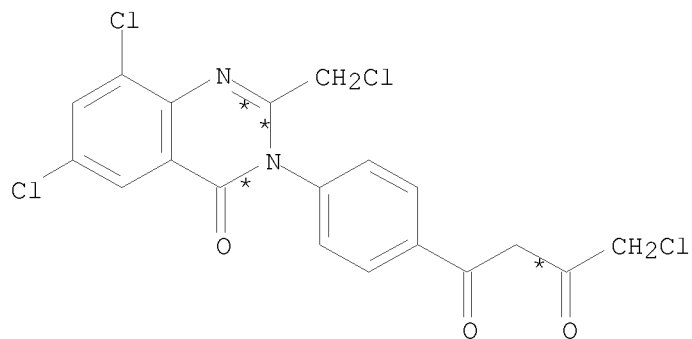


B



T

2  
STEPS  
=>



AA  
YIELD 49%

RX(4) RCT L 39263-98-4, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13  
SOL 108-88-3 PhMe  
CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

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STAGE(3)

RGT E 144-55-8 NaHCO3  
SOL 7732-18-5 Water  
CON neutralized

PRO M 748166-01-0

RX(9) RCT T 105-39-5

STAGE(1)

RGT V 124-41-4 NaOMe  
SOL 67-56-1 MeOH, 108-20-3 Isopropyl ether  
CON 5 minutes, room temperature

STAGE(2)

RCT M 748166-01-0  
SOL 108-20-3 Isopropyl ether  
CON SUBSTAGE(1) 5 minutes, room temperature  
SUBSTAGE(2) 24 hours, reflux

STAGE(3)

RGT W 7647-01-0 HCl  
SOL 7732-18-5 Water

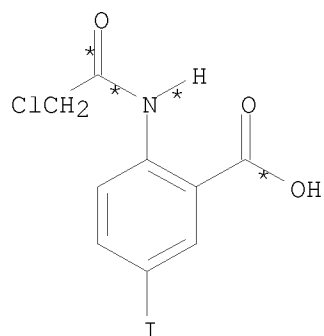
STAGE(4)

RGT X 497-19-8 Na2CO3  
SOL 7732-18-5 Water  
CON neutralized

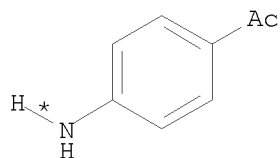
PRO AA 748166-06-5

RX(17) OF 17 COMPOSED OF RX(5), RX(10)

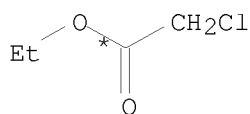
RX(17) N + B + T ==> AB



N



B



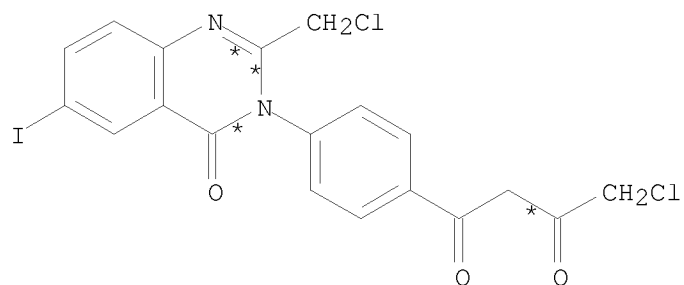
T

2

STEPS



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AB  
YIELD 63%

RX(5) RCT N 175850-45-0, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT E 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water

CON neutralized

PRO O 748166-02-1

RX(10) RCT T 105-39-5

STAGE(1)

RGT V 124-41-4 NaOMe

SOL 67-56-1 MeOH, 108-20-3 Isopropyl ether

CON 5 minutes, room temperature

STAGE(2)

RCT O 748166-02-1

SOL 108-20-3 Isopropyl ether

CON SUBSTAGE(1) 5 minutes, room temperature

SUBSTAGE(2) 24 hours, reflux

STAGE(3)

RGT W 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(4)

RGT X 497-19-8 Na<sub>2</sub>CO<sub>3</sub>

SOL 7732-18-5 Water

CON neutralized

PRO AB 748166-07-6

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 72 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 141:225304 CASREACT  
 TITLE: Preparation of cyclohexyl-substituted lactams as  
 cytokine receptor modulating agents  
 INVENTOR(S): Cherney, Robert J.; Carter, Percy; Duncia, John V.;  
 Gardner, Daniel S.; Santella, Joseph B.  
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA  
 SOURCE: PCT Int. Appl., 385 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

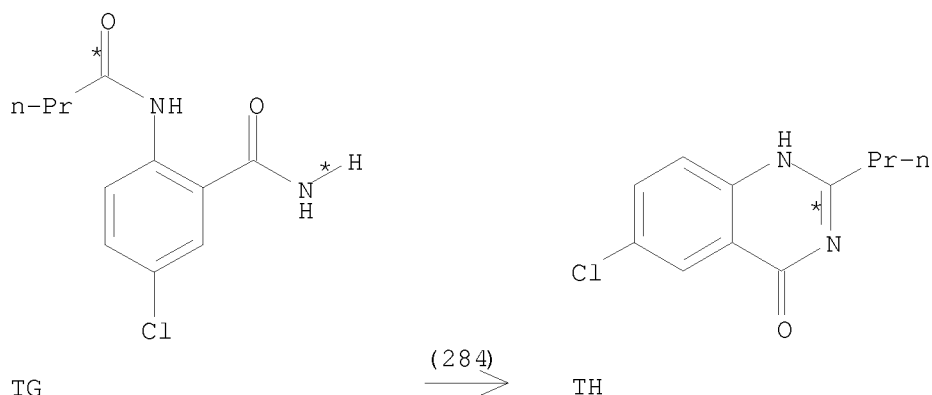
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004071460	A2	20040826	WO 2004-US4418	20040211
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20040186140	A1	20040923	US 2004-776828	20040211
US 7183270	B2	20070227		
EP 1606255	A2	20051221	EP 2004-710294	20040211
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 20070032541	A1	20070208	US 2006-545584	20061010
US 7338947	B2	20080304		
US 20080114052	A1	20080515	US 2008-18266	20080123
PRIORITY APPLN. INFO.:				
			US 2003-446850P	20030212
			US 2004-776828	20040211
			WO 2004-US4418	20040211
			US 2006-545584	20061010
OTHER SOURCE(S): MARPAT 141:225304				
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Cyclohexyl-substituted lactams I [A = (un)substituted saturated or partially saturated cycloalkyl or heterocycloalkyl group with 3-8 atoms; E = S(:O)pCHR3, CHR3NR3, C(:O)NR3, N(R3)C(:O)NR3, SO2N(R3), N(R3)SO2N(R3); G = (CHR10)n; J = CH2CH2, CH:CH un(substituted) with (R13)s; R1, R2 = (un)substituted aryl or heteroaryl ring; R3 = H, alkyl; R10 = H, (un)substituted alkyl (two R10 groups may together comprise a carbonyl group); R11, R12 (independently) = H, (un)substituted alkyl, aralkyl, heteroaralkyl, ε-hydroxyalkyl, ε-mercaptoalkyl, ε-alkoxyalkyl, etc.; R13 = H, (un)substituted alkyl; X = O, S; Z = bond, (un)substituted aminocarbonyl, aminothiocarbonyl, aminocarbonylamino, aminothiocarbonylamino, aminosulfonyl, aminosulfonylamino, carbonylamino, oxycarbonylamino,

aminocarbonyloxy, alkenediyl, methylene, etc.;  $m = 0-1$ ;  $n = 0-3$ ;  $s = 0-1$ ] such as II are prepared as modulators of cytokine activity for the treatment of diseases associated with cytokines and their receptors such as inflammation, osteo- and rheumatoid arthritis, autoimmune diseases, HIV infection, inflammatory bowel disease, asthma, multiple sclerosis, and atherosclerosis. E.g., 1,4-cyclohexanedione mono(ethylene ketal) is lithiated and acylated with Et cyanoformate, reductively aminated with (S)- $\alpha$ -methylbenzylamine, subjected to reduction with lithium aluminum hydride followed by hydrogenolysis with palladium hydroxide and protection with Cbz anhydride to yield nonracemic III. E.g., III undergoes substitution at the primary carbon with 4-bromophenyl disulfide and tributylphosphine followed by oxidation with mCPBA, Stille methylation of the p-bromophenyl moiety, hydrogenolysis of the Cbz protecting group, acylation with N-Cbz-L-methionine, and S-methylation and cyclization with Me iodide and cesium carbonate to yield IV. E.g., IV undergoes acid-catalyzed deketalization, titanium-mediated Meerwein-Ponndorf-Verley reduction with isopropylamine (giving a mixture of both epimers at the amine center), N-methylation with formaldehyde and sodium triacetoxyborohydride, hydrogenolysis of the Cbz protecting group on the aminopyrrolidinone, and acylation with 3-trifluoromethylbenzoic acid and HATU to yield II. The compds. are modulators of chemokine receptor activity (no data). In addition, methods of halolactamization and dehalogenation and reagents appropriate for such transformations are claimed.

RX(284) OF 1483 ...TG ==> TH...



RX(284) RCT TG 746671-46-5

STAGE(1)

RGT BD 1310-73-2 NaOH  
SOL 7732-18-5 Water, 64-17-5 EtOH  
CON 15 minutes, room temperature

STAGE(2)

RGT CL 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature, pH 2

PRO TH 69729-73-3

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REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 73 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 141:106431 CASREACT

TITLE: Synthesis of 6-bromomethyl-3,4-dihydro-2-methyl-4-oxoquinazoline

AUTHOR(S): Cao, Sheng-li; Ma, Xue-qin

CORPORATE SOURCE: Department of Chemistry, Capital Normal University, Beijing, 100037, Peop. Rep. China

SOURCE: Huaxue Shiji (2004), 26(1), 27-28, 49

CODEN: HUSHDR; ISSN: 0258-3283

PUBLISHER: Huagongbu Huaxue Shiji Xinsizhan

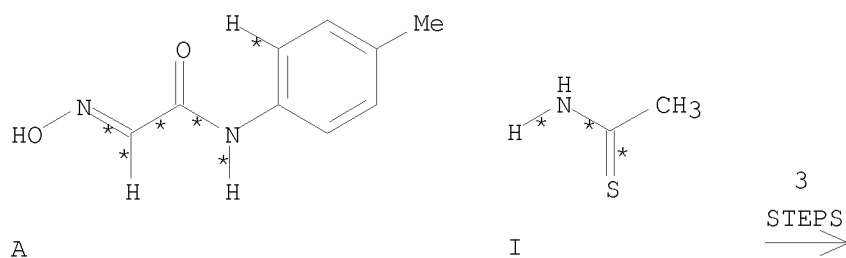
DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB Cyclization of 4-MeC<sub>6</sub>H<sub>4</sub>NHCOCH:NOH with H<sub>2</sub>SO<sub>4</sub> gave 5-methylisatin, oxidation of which with 30% H<sub>2</sub>O<sub>2</sub> gave 2-amino-5-methylbenzoic acid. Then, heating 2-amino-5-methylbenzoic acid with thioacetamide yielded 3,4-dihydro-2,6-dimethyl-4-oxoquinazoline which was brominated with N-bromosuccinimide in the presence of benzoyl peroxide to give the title compound in 23.1% overall yield.

RX(8) OF 10 COMPOSED OF RX(1), RX(2), RX(3)

RX(8) A + I ==> J



J  
YIELD 73%

RX(1) RCT A 1132-40-7  
RGT C 7664-93-9 H<sub>2</sub>SO<sub>4</sub>  
PRO B 608-05-9

RX(2) RCT B 608-05-9

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STAGE(1)

RGT E 7722-84-1 H2O2, F 1310-73-2 NaOH  
SOL 7732-18-5 Water  
CON 0.5 hours, 15 - 20 deg C

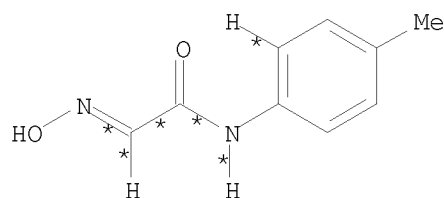
STAGE(2)

RGT G 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 0 deg C, pH 5 - 6

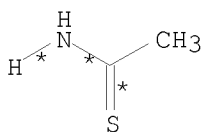
PRO D 2941-78-8

RX(3) RCT D 2941-78-8, I 62-55-5  
PRO J 18731-19-6  
CON 2 hours, 135 - 150 deg C

RX(10) OF 10 COMPOSED OF RX(1), RX(2), RX(3), RX(4)  
RX(10) A + I ==> K

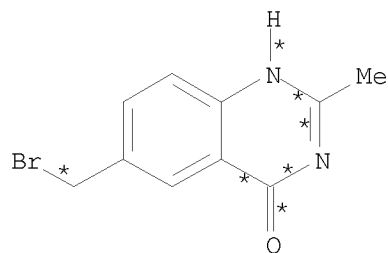


A



I

4  
STEPS  
→



K  
YIELD 76%

RX(1) RCT A 1132-40-7  
RGT C 7664-93-9 H2SO4  
PRO B 608-05-9

RX(2) RCT B 608-05-9

STAGE(1)

RGT E 7722-84-1 H2O2, F 1310-73-2 NaOH  
SOL 7732-18-5 Water  
CON 0.5 hours, 15 - 20 deg C

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STAGE(2)

RGT G 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 0 deg C, pH 5 - 6

PRO D 2941-78-8

RX(3) RCT D 2941-78-8, I 62-55-5  
PRO J 18731-19-6  
CON 2 hours, 135 - 150 deg C

RX(4) RCT J 18731-19-6  
RGT L 128-08-5 Bromosuccinimide  
PRO K 112888-43-4  
CAT 94-36-0 Benzoyl peroxide  
SOL 67-66-3 CHCl3  
CON 3 hours, 60 - 62 deg C  
NTE photochem.

L3 ANSWER 74 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 141:23764 CASREACT

TITLE: Facile zeolite induced Fischer-indole synthesis: a new approach to bioactive natural product rutaecarpine

AUTHOR(S): Mhaske, Santosh B.; Argade, Narshinha P.

CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National Chemical Laboratory, Pashan, Pune, 411 008, India

SOURCE: Tetrahedron (2004), 60(15), 3417-3420

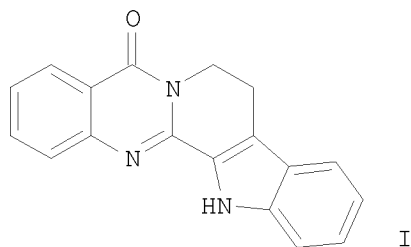
CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

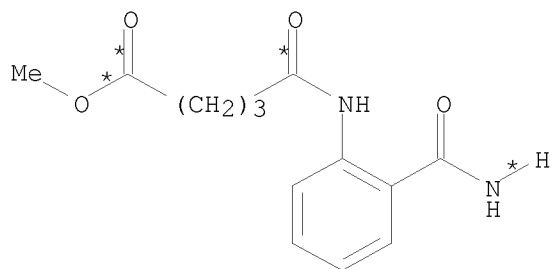


AB Starting from glutaric anhydride we have demonstrated an elegant six-step practical synthesis of bioactive natural product rutaecarpine (I) via o-amidoglutaranilic acid formation, esterification, chemoselective ester reduction, intramol. dehydrative cyclizations, hydrazone formation and zeolite induced Fischer-indole synthesis with 53% overall yield. The conditions employed in the present synthesis are mild, efficient and general.

RX(3) OF 21 ...G ==> I...

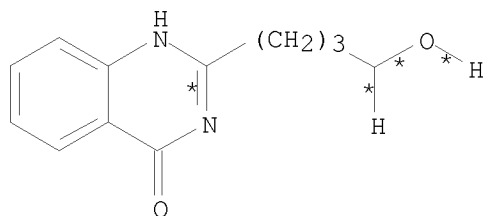


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G

(3)  $\longrightarrow$



I

YIELD 86%

RX(3) RCT G 697236-30-9

STAGE(1)

RGT J 16940-66-2 NaBH<sub>4</sub>

SOL 109-99-9 THF

CON 3 hours, reflux

STAGE(2)

RGT K 7732-18-5 Water

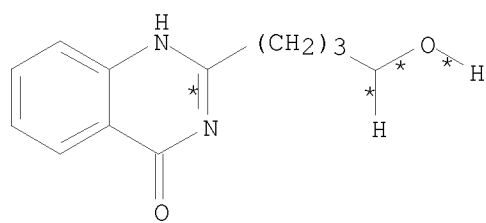
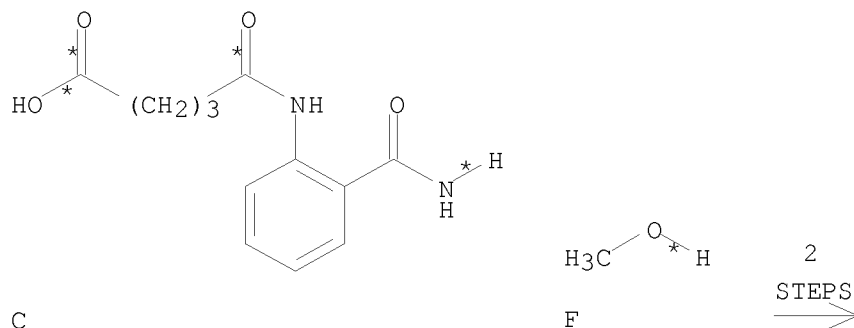
CON room temperature

PRO I 60915-16-4

RX(8) OF 21 COMPOSED OF RX(2), RX(3)

RX(8) C + F ==> I

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YIELD 86%

RX(2) RCT C 197236-49-0, F 67-56-1  
PRO G 697236-30-9  
CAT 7664-93-9 H2SO4  
SOL 67-56-1 MeOH  
CON 8 hours, room temperature

RX(3) RCT G 697236-30-9

STAGE(1)

RGT J 16940-66-2 NaBH4  
SOL 109-99-9 THF  
CON 3 hours, reflux

STAGE(2)

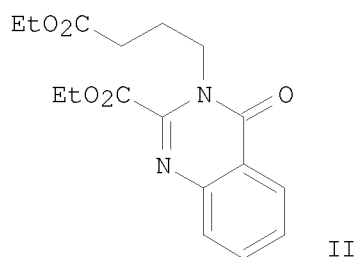
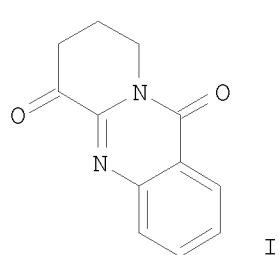
RGT K 7732-18-5 Water  
CON room temperature

PRO I 60915-16-4

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

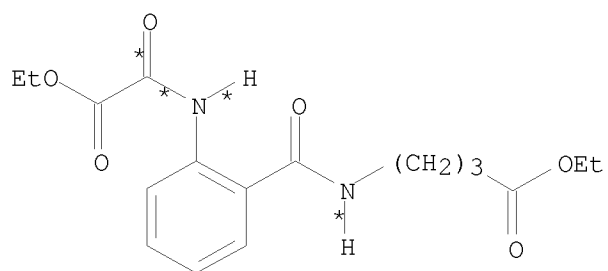
L3 ANSWER 75 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 141:7327 CASREACT  
TITLE: A facile total synthesis of rutaecarpine  
AUTHOR(S): Chavan, Subhash P.; Sivappa, R.  
CORPORATE SOURCE: Division of Organic Chemistry: Technology, National

SOURCE: Chemical Laboratory, Pune, 411-008, India  
 Tetrahedron Letters (2004), 45(5), 997-999  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

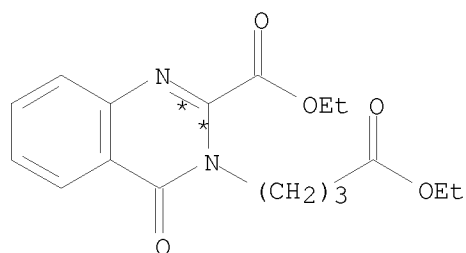


AB The indoloquinazoline alkaloid rutaecarpine was synthesized efficiently by employing 9,10,11,12-tetrahydro-4H-pyrido[2,1-b]quinazoline-4,9-dione (I) as a key intermediate, which was prepared by adapting a Dieckmann condensation-decarboxylation sequence from quinazolinone diester II.

RX(7) OF 29      ...Q ==> H...



(7)  $\longrightarrow$

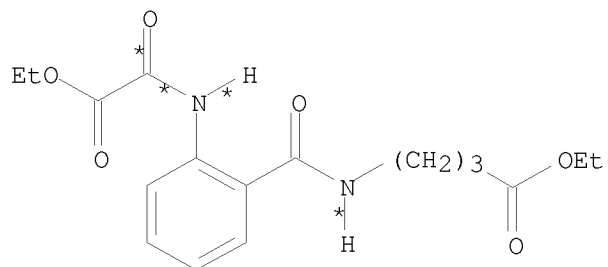


YIELD 80%

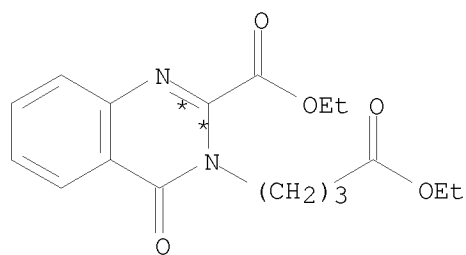
10/ 562,112

RX(7)      RCT    Q 693226-79-8  
             RGT    T 7719-12-2 PC13  
             PRO    H 107466-57-9  
             SOL    1330-20-7 Xylene  
             CON    2 hours, reflux

RX(8) OF 29      Q    ==>    H



Q



H  
YIELD 70%

RX(8)      RCT    Q 693226-79-8

STAGE(1)

RGT    V 603-35-0 PPh3, W 7553-56-2 I2, N 121-44-8 Et3N  
SOL    75-09-2 CH2Cl2

STAGE(2)

RGT    X 110-89-4 Piperidine  
SOL    75-05-8 MeCN  
CON    reflux

PRO    H 107466-57-9

REFERENCE COUNT:            27      THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 76 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 141:7091 CASREACT

TITLE: An interaction of 2-thiazoleacetonitriles with  
N-(2-chloroacetyl)anthranilic acid esterAUTHOR(S): Resnyanska, Elizaveta V.; Tverdokhlebov, Anton V.;  
Tolmachev, Andrey A.; Volovenko, Yulian M.; Shokol,  
Tatyana V.

CORPORATE SOURCE: Enamine Ltd. Co., Kiev, 02042, Ukraine

SOURCE: Heterocycles (2004), 63(4), 797-807

CODEN: HTCYAM; ISSN: 0385-5414

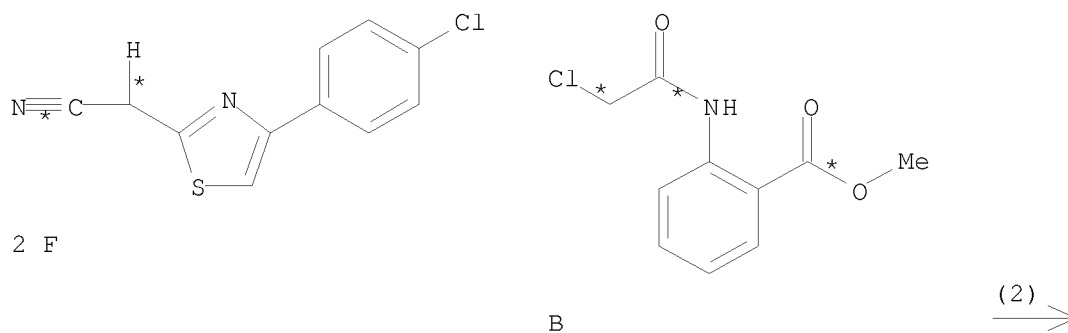
PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The title ester was found to react with 2-benzothiazoleacetonitrile yielding 3-(2-benzothiazolyl)-2,4-dihydropyrrolo[1,2-a]quinazoline-1,5-dione. At the same time 4-aryl-2-thiazoleacetonitriles gave 3,4-dihydro- $\beta$ ,4-dioxo- $\alpha$ , $\delta$ -bis(4-aryl-2-thiazolyl)-2-quinazolinepentanenitriles potassium salts under identical conditions. These results were explained in terms of different solubility of the intermediate compds. Upon acidification the obtained salts were shown to undergo intramol. Thorpe addition leading to the 3-amino-2,4-bis(4-aryl-2-thiazolyl)-4-[4(3H)-oxo-2-quinazolinyl]-2-cyclopenten-1-ones. Above mentioned pyrrolo[1,2-a]quinazoline derivative was treated with benzylamines and active methylene nitriles to yield  $\beta$ -(2-benzothiazolyl)-N-arylmethyl-3,4-dihydro-4-oxo-2-quinazolinepropanamides and 2-substituted 3-amino-4-(2-benzothiazolyl)-4-[4(3H)-oxo-2-quinazolinyl]-2-cyclopenten-1-ones, resp.

RX(2) OF 15 2 F + B ==&gt; G...



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT F 17969-48-1, B 58915-18-7

RGT D 584-08-7 K2CO3

PRO G 694495-39-1

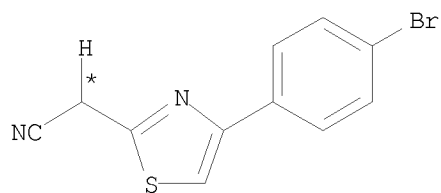
SOL 64-17-5 EtOH

CON 1.5 hours, reflux

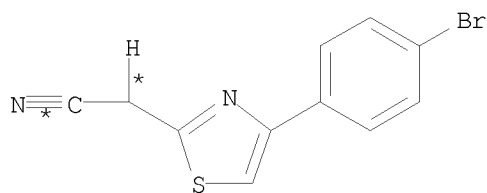
NTE Claisen type acylation

RX(3) OF 15 2 H + B ==&gt; I...

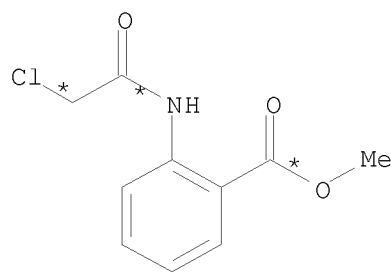
10/ 562,112



H



H



B

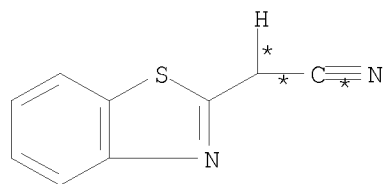


\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

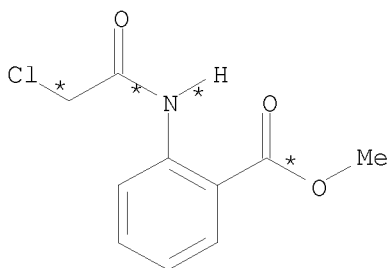
RX(3) RCT H 94833-31-5, B 58915-18-7  
 RGT D 584-08-7 K2CO3  
 PRO I 694495-40-4  
 SOL 64-17-5 EtOH  
 CON 1.5 hours, reflux  
 NTE Claisen type acylation

RX(12) OF 15 COMPOSED OF RX(1), RX(8)

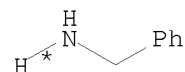
RX(12) A + B + S ==> T



A



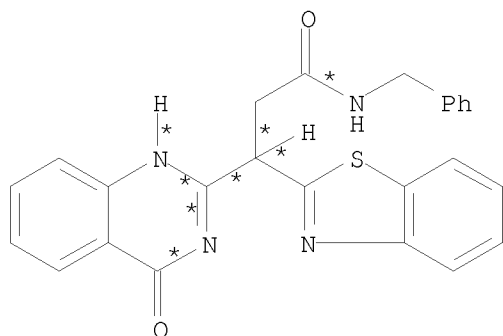
B



S

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2  
STEPS  
→

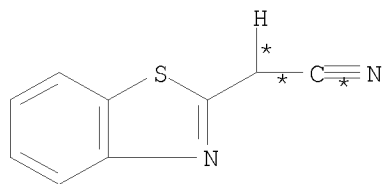


T  
YIELD 54%

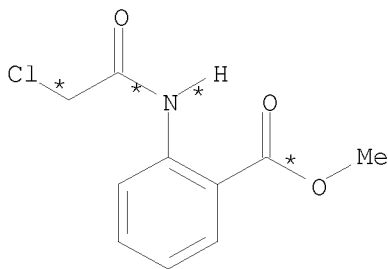
RX(1) RCT A 56278-50-3, B 58915-18-7  
RGT D 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO C 519048-05-6  
SOL 64-17-5 EtOH  
CON 1.5 hours, reflux

RX(8) RCT S 100-46-9, C 519048-05-6  
PRO T 565179-87-5  
SOL 68-12-2 DMF  
CON 3 hours, 100 deg C

RX(13) OF 15 COMPOSED OF RX(1), RX(9)  
RX(13) A + B + U ==> V

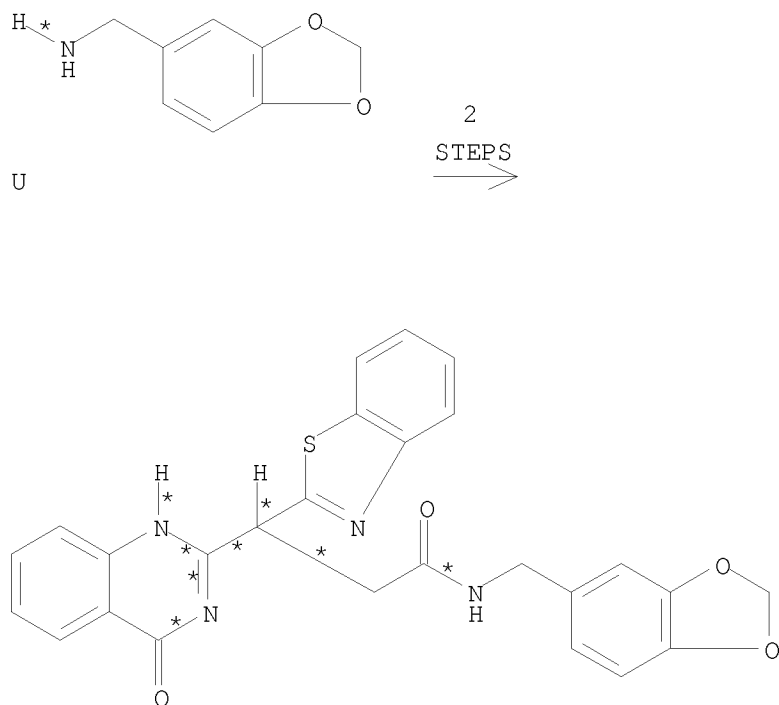


A



B

10/ 562,112



V  
YIELD 56%

RX(1) RCT A 56278-50-3, B 58915-18-7  
RGT D 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO C 519048-05-6  
SOL 64-17-5 EtOH  
CON 1.5 hours, reflux

RX(9) RCT U 2620-50-0, C 519048-05-6  
PRO V 568577-53-7  
SOL 68-12-2 DMF  
CON 3 hours, 100 deg C

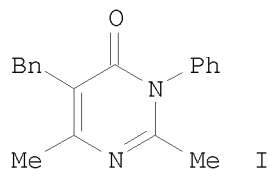
REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 77 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 140:339284 CASREACT  
TITLE: An efficient synthesis of 3-substituted 3H-pyrimidin-4-ones  
AUTHOR(S): Jeong, Jae Uk; Chen, Xiaohong; Rahman, Attiq; Yamashita, Dennis S.; Luengo, Juan I.  
CORPORATE SOURCE: Department of Medicinal Chemistry, MMPD CEDD, GlaxoSmithKline, Collegeville, PA, 19426, USA  
SOURCE: Organic Letters (2004), 6(6), 1013-1016  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society



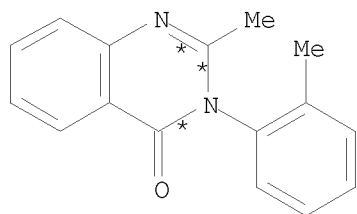
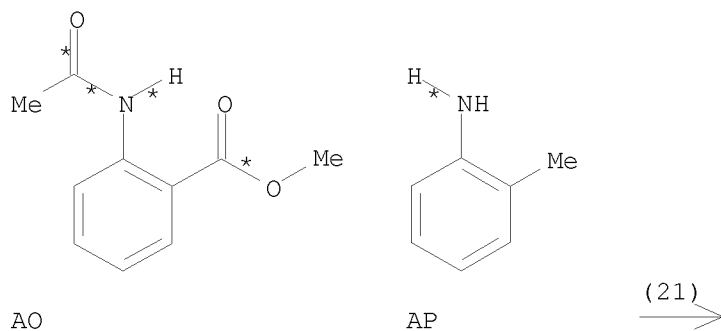
10/ 562,112

DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB A practical synthesis of 3-substituted 3H-pyrimidin-4-ones, e.g., I, is described. The key step involved the cyclization of enamide esters, derived from readily available  $\beta$ -keto esters, with various primary amines.

RX(21) OF 42 AO + AP ==> AQ



AQ  
YIELD 72%

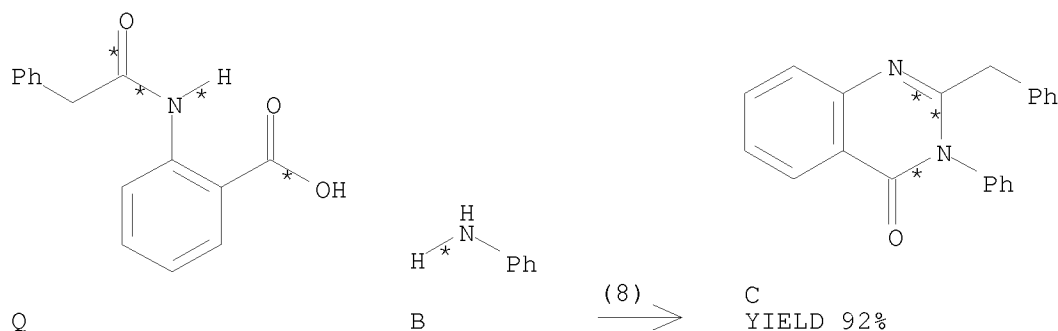
RX(21) RCT AO 2719-08-6, AP 95-53-4  
RGT P 75-24-1 AlMe<sub>3</sub>  
PRO AQ 72-44-6  
SOL 107-06-2 ClCH<sub>2</sub>CH<sub>2</sub>Cl  
CON 18 hours, reflux

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 78 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 140:321321 CASREACT  
 TITLE: Eco-friendly synthesis of quinazolin-4(3H)-ones  
 AUTHOR(S): Kidwai, Mazaahir; Ruby; Rastogi, Shweta  
 CORPORATE SOURCE: Department of Chemistry, University of Delhi, Delhi, 110 007, India  
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2004), 43B(2), 423-425  
 CODEN: IJSBDB; ISSN: 0376-4699  
 PUBLISHER: National Institute of Science Communication  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

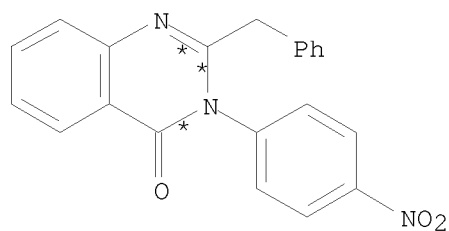
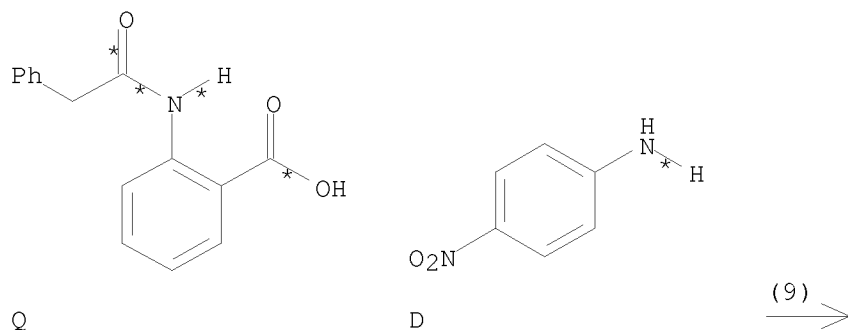
AB Several substituted quinazolin-4(3H)-ones were synthesized using environmentally benign procedure. Neat reactants on subjecting to microwave irradiation in the presence of dicyclohexylcarbodiimide as a condensing agent give the required products more quickly and in better yields in comparison to traditional methodologies. The observed yields and enhancement in reaction rates were due to the solvent-free conditions coupled with microwave usage.

RX(8) OF 14 Q + B ==> C



RX(8) RCT Q 28565-98-2, B 62-53-3  
 RGT R 538-75-0 DCC  
 PRO C 19857-34-2  
 CON 2.5 minutes  
 NTE microwave irradiation, alternative preparation shown, no solvent

RX(9) OF 14 Q + D ==> E



YIELD 93%

RX(9) RCT Q 28565-98-2, D 100-01-6  
 RGT R 538-75-0 DCC  
 PRO E 201293-05-2  
 CON 3 minutes  
 NTE microwave irradiation, alternative preparation shown, no solvent

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 79 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 140:321181 CASREACT

TITLE: First Reported Nonpeptide AT1 Receptor Agonist (L-162,313) Acts as an AT2 Receptor Agonist in Vivo

AUTHOR(S): Wan, Yiqian; Wallinder, Charlotta; Johansson, Berndt; Holm, Mathias; Mahalingam, A. K.; Wu, Xiongyu; Botros, Milad; Karlen, Anders; Pettersson, Anders; Nyberg, Fred; Faendriks, Lars; Hallberg, Anders; Alterman, Mathias

CORPORATE SOURCE: Department of Medicinal Chemistry BMC, Uppsala University, Uppsala, SE-751 23, Swed.

SOURCE: Journal of Medicinal Chemistry (2004), 47(6), 1536-1546

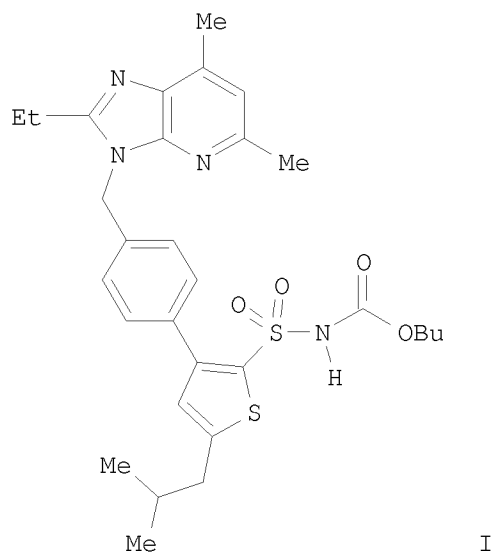
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

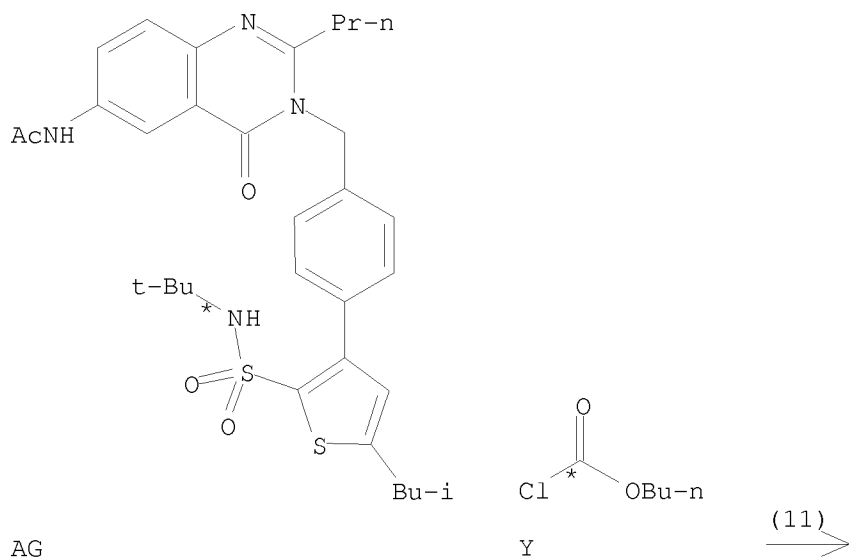
DOCUMENT TYPE: Journal

LANGUAGE: English

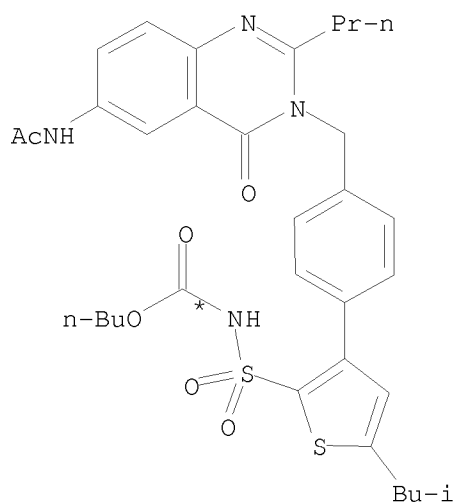
GI



AB In this investigation, it is demonstrated that the first nonpeptide AT1 receptor agonist L-162,313 (I), disclosed in 1994, also acts as an agonist at the AT2 receptor. In anesthetized rats, administration of compound I i.v. or locally in the duodenum increased duodenal mucosal alkaline secretion, effects that were sensitive to the selective AT2 receptor antagonist PD-123,319. The data strongly suggest that I is an AT2 receptor agonist in vivo. To the best of our knowledge, this substance is the first nonpeptidic low-mol. weight compound with an agonistic effect mediated through the AT2 receptor.

$$\text{RX(11) OF 101} \quad \dots \text{AG} + \text{Y} \implies \text{AJ}$$


10/ 562,112



AJ  
YIELD 71%

RX(11) RCT AG 678144-78-0

STAGE(1)

RGT D 100-66-3 PhOMe

SOL 76-05-1 F3CCO2H, 7732-18-5 Water

CON overnight, room temperature

STAGE(2)

RCT Y 592-34-7

RGT E 2456-81-7 4-Pyrrolidino-py

SOL 110-86-1 Pyridine

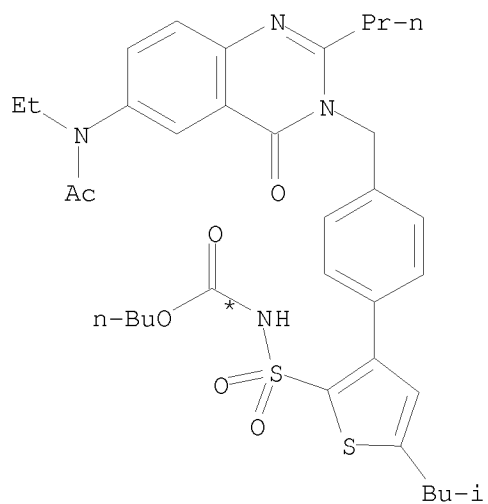
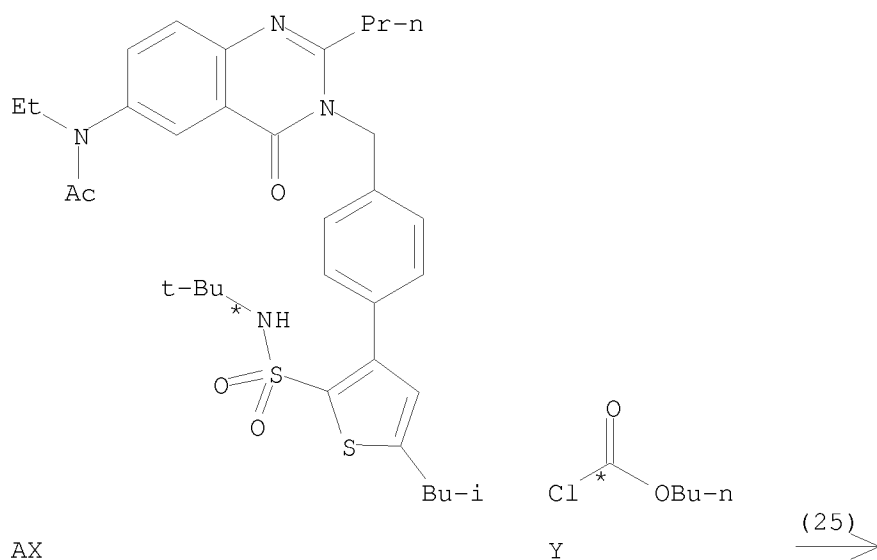
CON SUBSTAGE(1) <room temperature

SUBSTAGE(2) overnight, room temperature

PRO AJ 678144-79-1

RX(25) OF 101 ...AX + Y ==> BE

10/ 562,112



BE  
YIELD 40%

RX(25) RCT AX 678144-91-7

STAGE(1)

RGT D 100-66-3 PhOMe  
SOL 76-05-1 F3CCO2H, 7732-18-5 Water  
CON overnight, room temperature

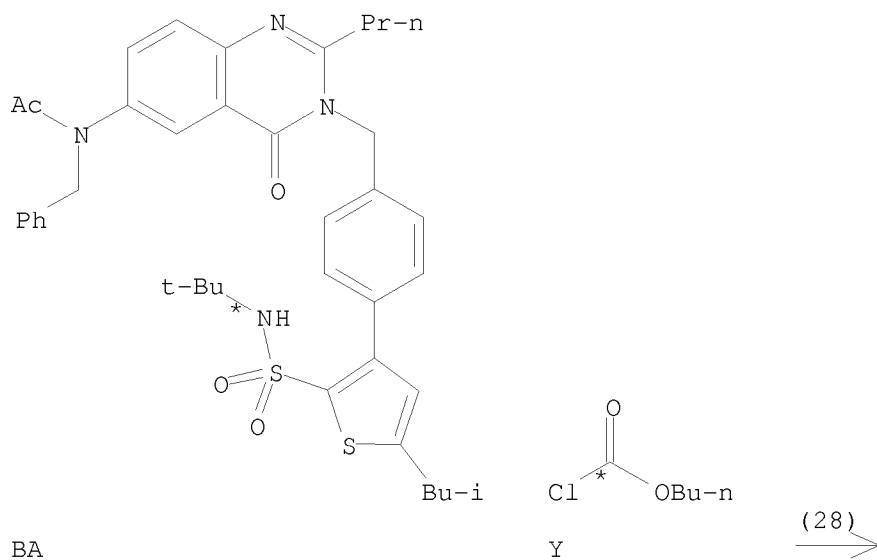
STAGE(2)

RCT Y 592-34-7  
RGT E 2456-81-7 4-Pyrrolidino-py  
SOL 110-86-1 Pyridine  
CON SUBSTAGE(1) <room temperature  
SUBSTAGE(2) overnight, room temperature

10/ 562,112

PRO BE 678144-99-5

RX(28) OF 101 ...BA + Y ==> BH



BH  
YIELD 77%

RX(28) RCT BA 678144-95-1

STAGE(1)

RGT D 100-66-3 PhOMe  
SOL 76-05-1 F3CCO2H, 7732-18-5 Water  
CON overnight, room temperature

10/ 562,112

STAGE(2)

RCT Y 592-34-7

RGT E 2456-81-7 4-Pyrrolidino-py

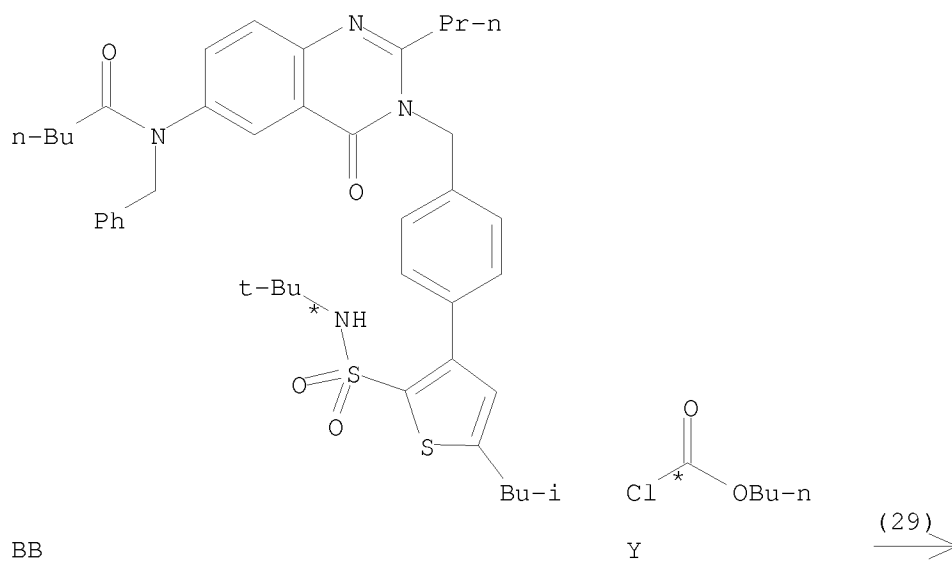
SOL 110-86-1 Pyridine

CON SUBSTAGE(1) <room temperature

SUBSTAGE(2) overnight, room temperature

PRO BH 678145-02-3

RX(29) OF 101 ...BB + Y ==> BI



BI  
YIELD 68%

RX(29) RCT BB 678144-96-2



STAGE(1)

RGT D 100-66-3 PhOMe  
SOL 76-05-1 F3CCO2H, 7732-18-5 Water  
CON overnight, room temperature

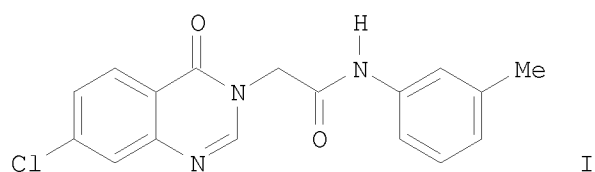
STAGE(2)

RCT Y 592-34-7  
RGT E 2456-81-7 4-Pyrrolidino-py  
SOL 110-86-1 Pyridine  
CON SUBSTAGE(1) <room temperature  
SUBSTAGE(2) overnight, room temperature

PRO BI 678145-03-4

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

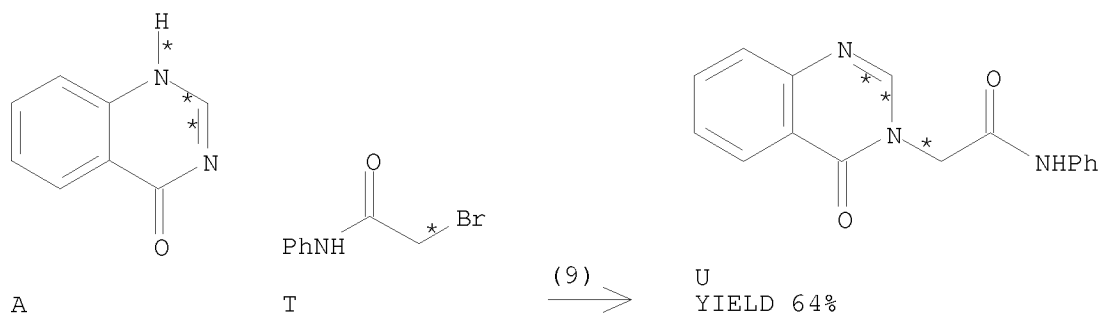
L3 ANSWER 80 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 140:253523 CASREACT  
TITLE: New 3-substituted quinazolin-4(3H)-one derivatives  
AUTHOR(S): Georgescu, E.; Georgescu, Florentina; Caproiu, M. T.; Draghici, C.  
CORPORATE SOURCE: "C.D. Nenitzescu" Institute of Organic Chemistry, Romanian Academy, Bucharest, Rom.  
SOURCE: Scientific Bulletin - University "Politehnica" of Bucharest, Series B: Chemistry and Materials Science (2002), 64(2), 27-38  
CODEN: SBUPBD; ISSN: 1454-2331  
PUBLISHER: University "Politehnica" of Bucharest  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB 3-Substituted quinazolin-4(3H)-one derivs., e.g., I, were obtained by condensation of quinazolin-4(3H)-ones with  $\alpha$ -halocarbonyl compds., such as  $\omega$ -bromo-2-acetyl thiophene and halo acetanilides, in the presence of sodium methoxide.

RX(9) OF 27 A + T ==> U

10/ 562,112



RX(9) RCT A 491-36-1

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

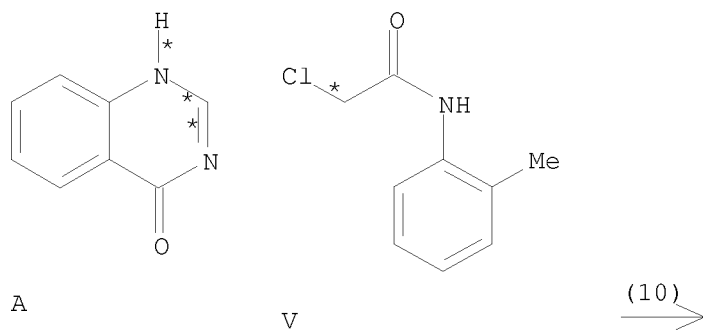
RCT T 5326-87-4

CON SUBSTAGE(1) 2 hours, reflux

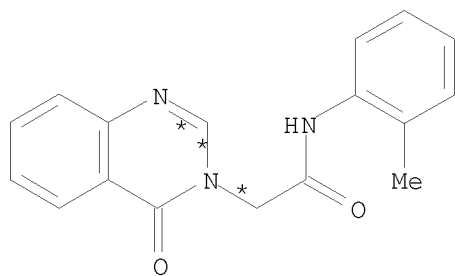
SUBSTAGE(2) overnight, cooled

PRO U 108086-38-0

RX(10) OF 27 A + V ==> W



10/ 562,112



W  
YIELD 68%

RX(10) RCT A 491-36-1

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

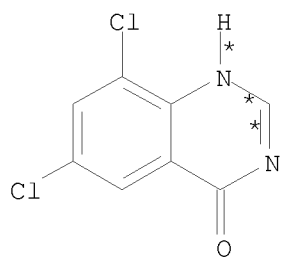
RCT V 37394-93-7

CON SUBSTAGE(1) 2 hours, reflux

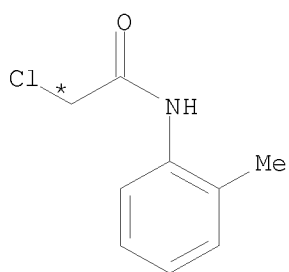
SUBSTAGE(2) overnight, cooled

PRO W 374640-63-8

RX(12) OF 27 P + V ==> Y



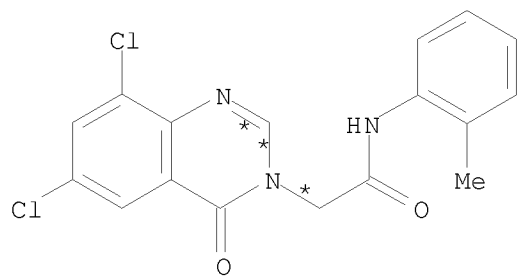
P



V

(12)  
→

10/ 562,112



Y  
YIELD 75%

RX(12) RCT P 6952-11-0

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

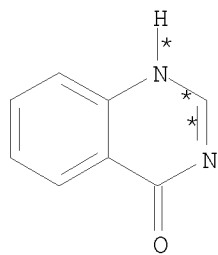
RCT V 37394-93-7

CON SUBSTAGE(1) 2 hours, reflux

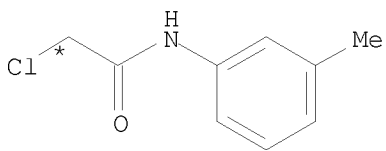
SUBSTAGE(2) overnight, cooled

PRO Y 374640-80-9

RX(13) OF 27 A + Z ==> AA



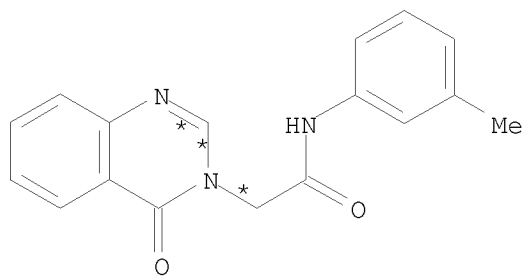
A



Z

(13)  $\longrightarrow$

10/ 562,112



AA  
YIELD 71%

RX(13) RCT A 491-36-1

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

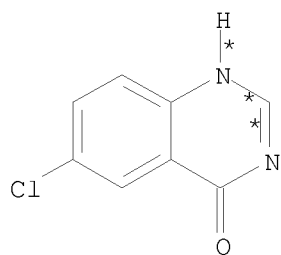
RCT Z 32428-61-8

CON SUBSTAGE(1) 2 hours, reflux

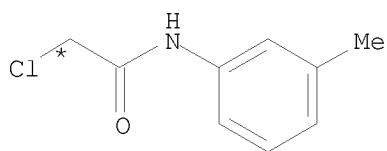
SUBSTAGE(2) overnight, cooled

PRO AA 353760-61-9

RX(14) OF 27 F + Z ==> AB



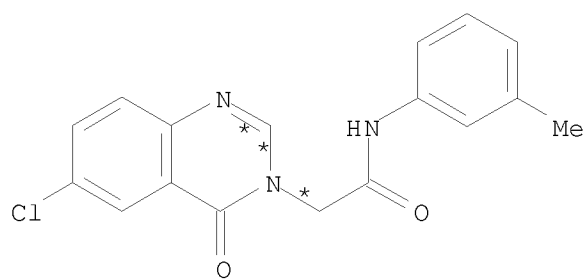
F



Z

(14)

10/ 562,112



AB  
YIELD 74%

RX(14) RCT F 16064-14-5

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

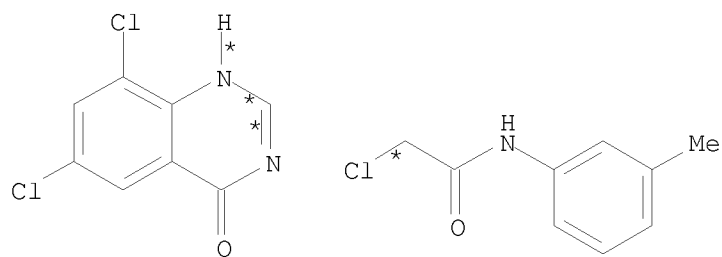
RCT Z 32428-61-8

CON SUBSTAGE(1) 2 hours, reflux

SUBSTAGE(2) overnight, cooled

PRO AB 374640-69-4

RX(16) OF 27 P + Z ==> AD

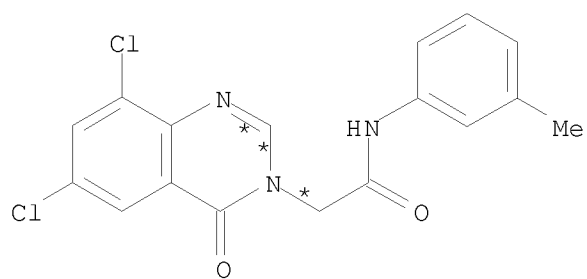


P

Z

(16)

10/ 562,112



AD  
YIELD 73%

RX(16) RCT P 6952-11-0

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

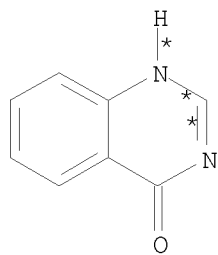
RCT Z 32428-61-8

CON SUBSTAGE(1) 2 hours, reflux

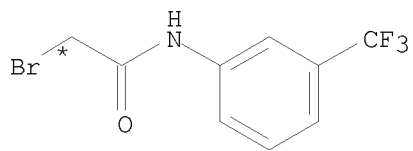
SUBSTAGE(2) overnight, cooled

PRO AD 374640-82-1

RX(17) OF 27 A + AE ==> AF



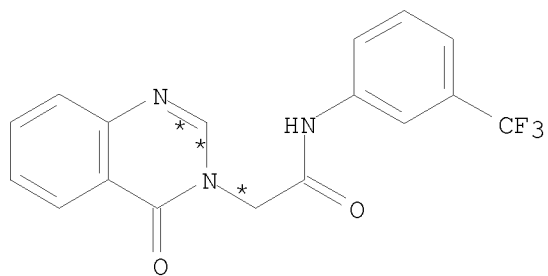
A



AE

(17)

10/ 562,112



AF  
YIELD 65%

RX(17) RCT A 491-36-1

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

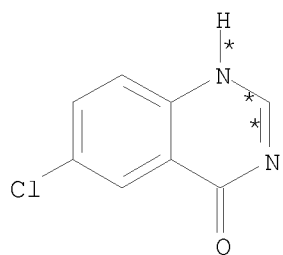
RCT AE 25625-57-4

CON SUBSTAGE(1) 2 hours, reflux

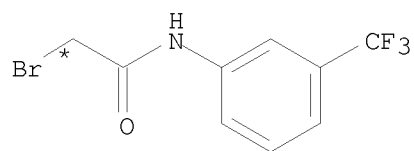
SUBSTAGE(2) overnight, cooled

PRO AF 361189-71-1

RX(18) OF 27 F + AE ==> AG



F

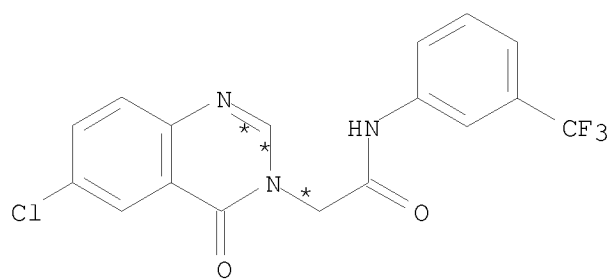


AE

(18)



10/ 562,112



AG  
YIELD 69%

RX(18) RCT F 16064-14-5

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

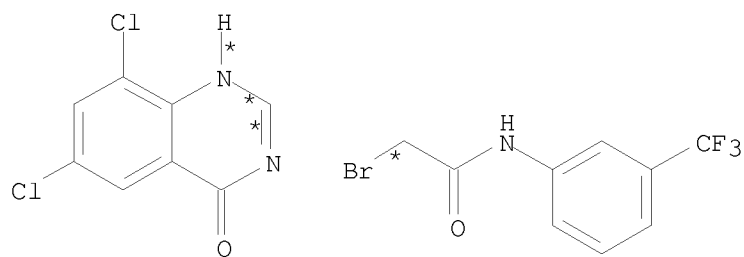
RCT AE 25625-57-4

CON SUBSTAGE(1) 2 hours, reflux

SUBSTAGE(2) overnight, cooled

PRO AG 374640-27-4

RX(20) OF 27 P + AE ==> AI

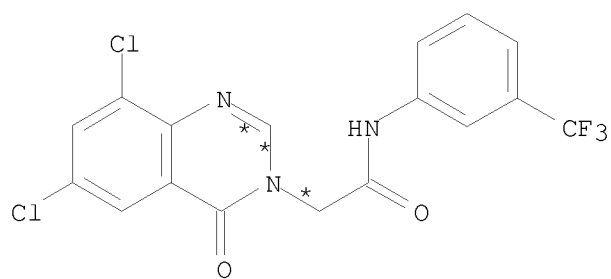


P

AE

(20)  
→

10/ 562,112



AI  
YIELD 68%

RX(20) RCT P 6952-11-0

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

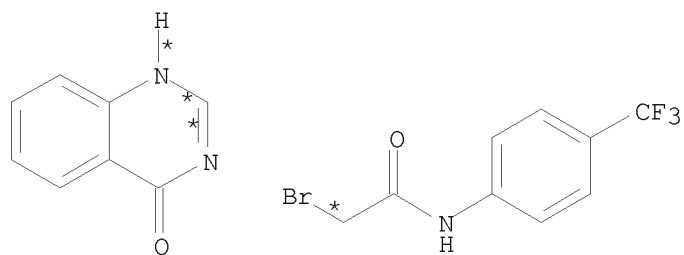
RCT AE 25625-57-4

CON SUBSTAGE(1) 2 hours, reflux

SUBSTAGE(2) overnight, cooled

PRO AI 374640-29-6

RX(21) OF 27 A + AJ ==> AK

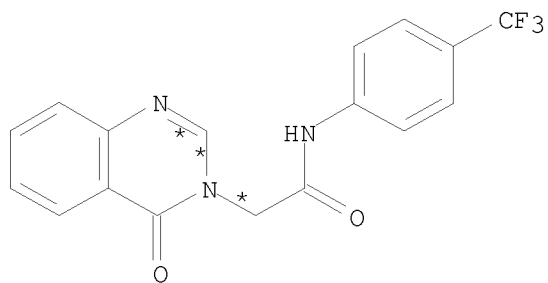


A

AJ

(21)

10/ 562,112



AK  
YIELD 71%

RX(21) RCT A 491-36-1

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

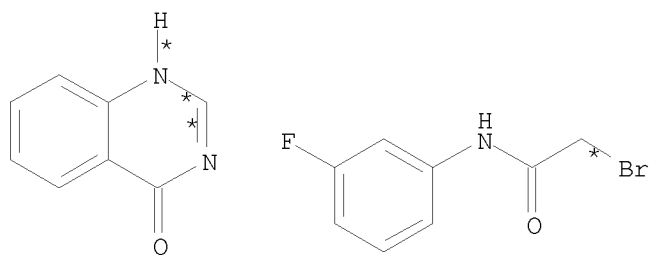
RCT AJ 3823-19-6

CON SUBSTAGE(1) 2 hours, reflux

SUBSTAGE(2) overnight, cooled

PRO AK 362492-98-6

RX(22) OF 27 A + AL ==> AM

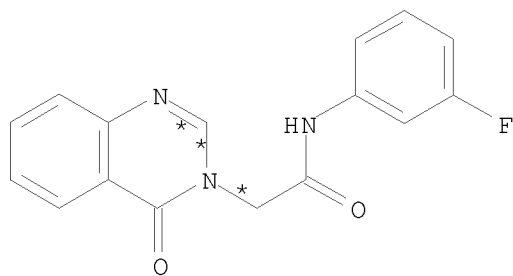


A

AL

(22)

10/ 562,112



AM  
YIELD 72%

RX(22) RCT A 491-36-1

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

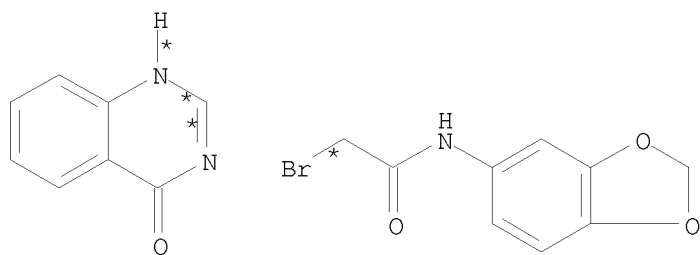
RCT AL 73392-04-8

CON SUBSTAGE(1) 2 hours, reflux

SUBSTAGE(2) overnight, cooled

PRO AM 361190-24-1

RX(23) OF 27 A + AN ==> AO

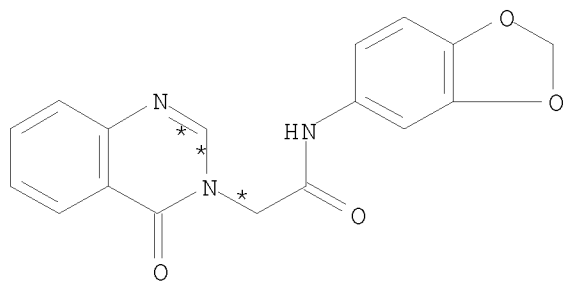


A

AN

(23)

10/ 562,112



AO  
YIELD 69%

RX(23) RCT A 491-36-1

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

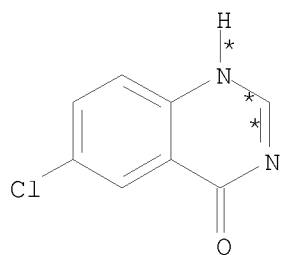
RCT AN 860806-13-9

CON SUBSTAGE(1) 2 hours, reflux

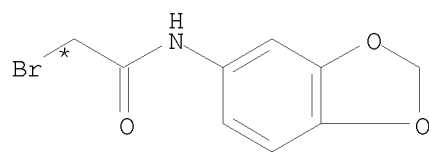
SUBSTAGE(2) overnight, cooled

PRO AO 374678-80-5

RX(24) OF 27 F + AN ==> AP



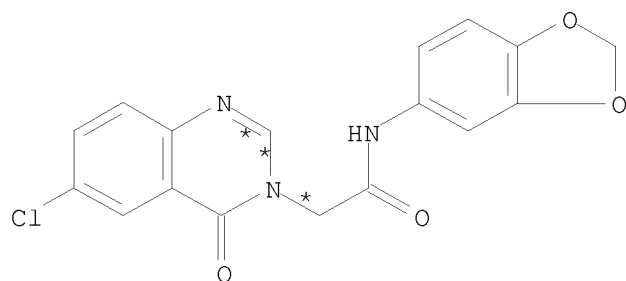
F



AN

(24)  
→

10/ 562,112



AP  
YIELD 65%

RX(24) RCT F 16064-14-5

STAGE(1)

RGT D 124-41-4 NaOMe  
SOL 67-56-1 MeOH  
CON 10 minutes, room temperature

STAGE(2)

RCT AN 860806-13-9  
CON SUBSTAGE(1) 2 hours, reflux  
SUBSTAGE(2) overnight, cooled

PRO AP 374678-81-6

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 81 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 140:181406 CASREACT

TITLE: Amine-induced rearrangement of  
4-imino-4H-3,1-benzoxazines to 4-quinazolinones via  
amidine carboxamides

AUTHOR(S): Snider, Barry B.; Zeng, Hongbo

CORPORATE SOURCE: Department of Chemistry MS 015, Brandeis University,  
Waltham, MA, 02454-9110, USA

SOURCE: Heterocycles (2003), 61, 173-182  
CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

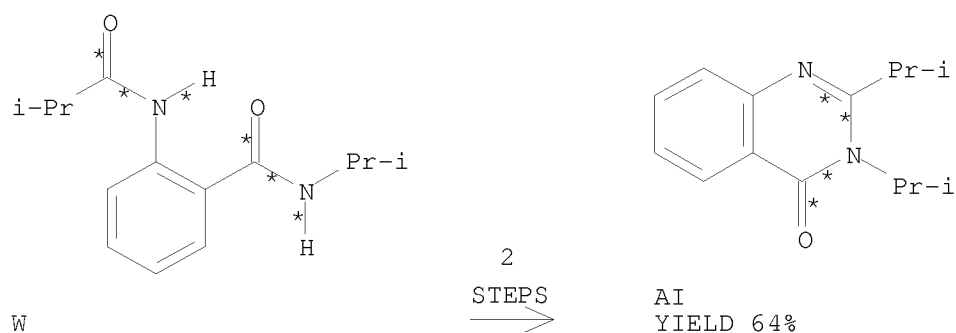
LANGUAGE: English

AB Iminobenzoxazines react with pyrrolidine in EtOAc at reflux to give  
amidine carboxamides, which cyclize to quinazolinones on heating in 99:1  
MeCN/HOAc. Some amidine intermediates could be isolated. A sterically  
hindered amidine does not cyclize to give the corresponding quinazolinone.

RX(27) OF 35 COMPOSED OF RX(8), RX(20)

RX(27) W ==> AI

10/ 562,112



RX(8)

STAGE(1)

RGT G 7726-95-6 Br<sub>2</sub>, H 603-35-0 PPh<sub>3</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0.5 hours, room temperature

STAGE(2)

RCT W 660425-84-3  
RGT I 121-44-8 Et<sub>3</sub>N  
CON 1.5 hours, reflux

STAGE(3)

RGT J 144-55-8 NaHCO<sub>3</sub>  
SOL 7732-18-5 Water

PRO X 660425-89-8

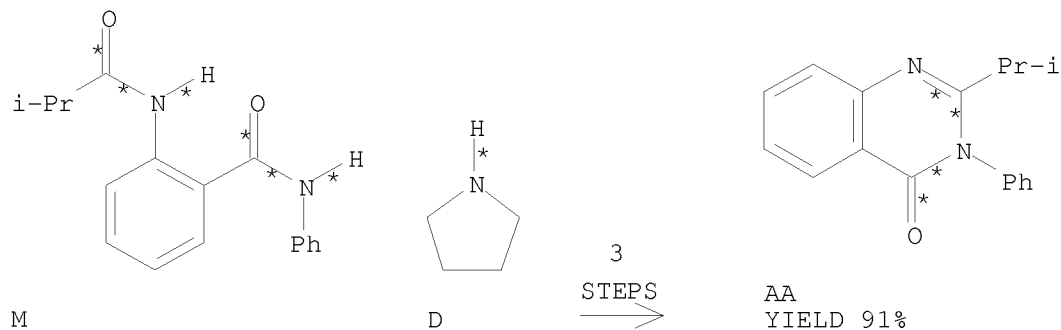
NTE mixture with 11 % of educt was isolated%

RX(20)

RCT X 660425-89-8  
RGT C 64-19-7 AcOH  
PRO AI 660425-96-7  
CAT 123-75-1 Pyrrolidine  
SOL 75-05-8 MeCN  
CON 36 hours, reflux  
NTE regioselective

RX(33) OF 35 COMPOSED OF RX(3), RX(11), RX(12)

RX(33) M + D ==> AA



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RX(3)

STAGE(1)

RGT G 7726-95-6 Br2, H 603-35-0 PPh3  
SOL 75-09-2 CH2Cl2  
CON 0.5 hours, room temperature

STAGE(2)

RCT M 38163-55-2  
RGT I 121-44-8 Et3N  
CON 1.5 hours, reflux

STAGE(3)

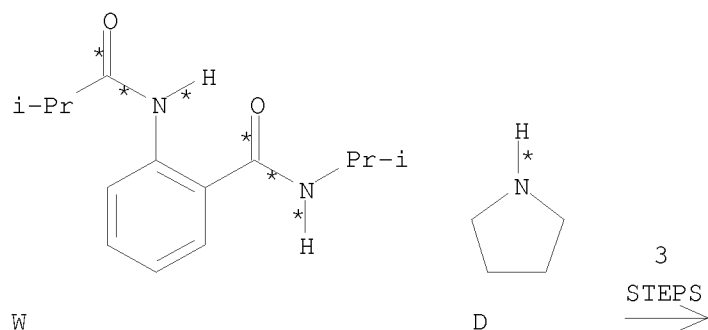
RGT J 144-55-8 NaHCO3  
SOL 7732-18-5 Water

PRO N 660425-85-4

RX(11) RCT N 660425-85-4, D 123-75-1  
PRO Z 660425-91-2  
SOL 123-75-1 Pyrrolidine  
CON 2 hours, 80 deg C  
NTE alternative reaction conditions gave lower yield, alternative  
reaction conditions shown

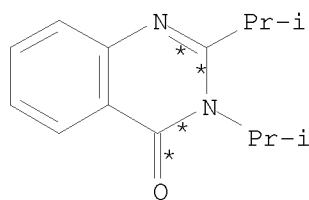
RX(12) RCT Z 660425-91-2  
PRO AA 32700-64-4  
CAT 64-19-7 AcOH  
SOL 75-05-8 MeCN  
CON 2 hours, reflux

RX(35) OF 35 COMPOSED OF RX(8), RX(17), RX(18)  
RX(35) W + D ==> AI





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AI  
YIELD 92%

RX(8)

STAGE(1)

RGT G 7726-95-6 Br<sub>2</sub>, H 603-35-0 PPh<sub>3</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 0.5 hours, room temperature

STAGE(2)

RCT W 660425-84-3  
RGT I 121-44-8 Et<sub>3</sub>N  
CON 1.5 hours, reflux

STAGE(3)

RGT J 144-55-8 NaHCO<sub>3</sub>  
SOL 7732-18-5 Water

PRO X 660425-89-8  
NTE mixture with 11 % of educt was isolated%

RX(17) RCT X 660425-89-8, D 123-75-1  
PRO AH 660425-95-6  
SOL 141-78-6 AcOEt  
CON 1.5 hours, 80 deg C  
NTE regioselective

RX(18) RCT AH 660425-95-6  
PRO AI 660425-96-7  
SOL 75-05-8 MeCN  
CON 10 hours, reflux  
NTE alternative reaction conditions gave lower yield, alternative reaction conditions shown

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 82 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 139:381438 CASREACT

TITLE: Various new types of macrocycles containing quinazolinone and tetrahydrobenzothienopyrimidinone rings with biological interest

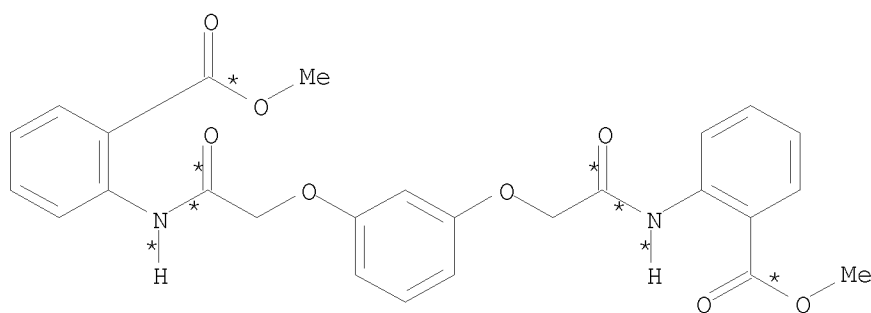
AUTHOR(S): El-Sharief, A. M. Sh.; Ammar, Y. A.; Zahran, M. A.; Ali, A. H.; El-Gaby, M. S. A.

CORPORATE SOURCE: Chemistry Department, Faculty of Science, Al-Azhar

SOURCE: University, Nasr City, Cairo, 11884, Egypt  
 Afinidad (2003), 60(503), 32-41  
 CODEN: AFINAE; ISSN: 0001-9704  
 PUBLISHER: Asociacion de Quimicos del Instituto Quimico de Sarria  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

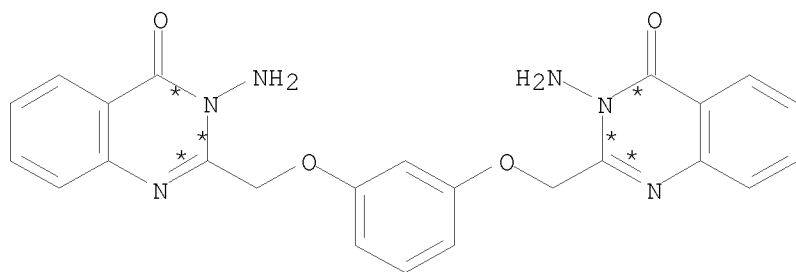
AB Synthesis and characterization of new aza crown type compds. are included by reacting the corresponding bis(3-amino quinazolinone) and bis(3-aminotetrahydrobenzothieno[2,3-d]pyrimidinone) with the resp. reagents. Most of these compds. were test in vitro for their antimicrobial activities against some gram pos. and gram neg. bacteria along with their antifungal activities.

RX(3) OF 67 ...I ==> L...



I

(3)  $\longrightarrow$

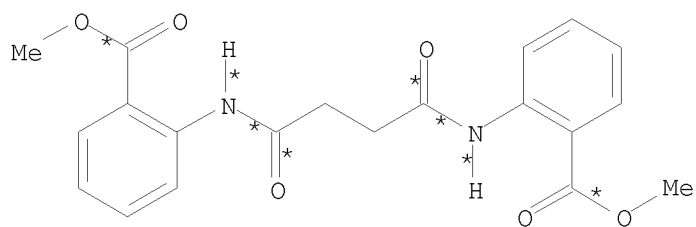


L  
 YIELD 85%

RX(3) RCT I 623928-01-8  
 RGT M 302-01-2 N2H4  
 PRO L 181770-29-6  
 SOL 71-36-3 BuOH  
 CON SUBSTAGE(1) 6 - 10 hours, reflux  
 SUBSTAGE(2) reflux -> 0 deg C

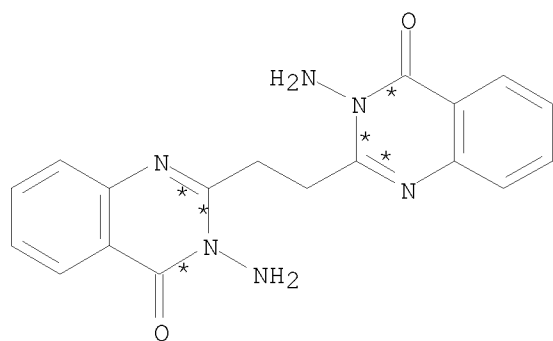
RX(13) OF 67 ...AD ==> AI...

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AD

(13)  $\longrightarrow$

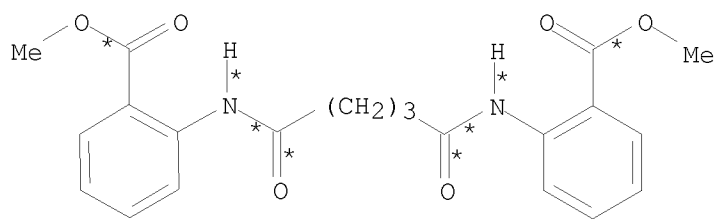


AI

YIELD 65%

RX(13)      RCT    AD 501938-94-9  
               RGT    M 302-01-2 N2H4  
               PRO    AI 623928-08-5  
               SOL    71-36-3 BuOH  
               CON    SUBSTAGE(1) 6 - 8 hours, reflux  
                       SUBSTAGE(2) reflux -> 0 deg C

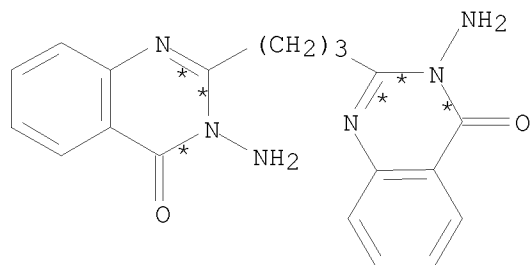
RX(14) OF 67      ...AF ==> AJ...



AF

(14)  $\longrightarrow$

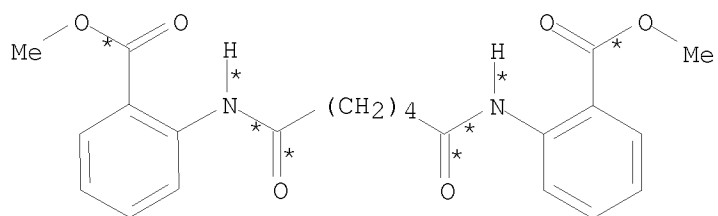
10/ 562,112



AJ  
YIELD 61%

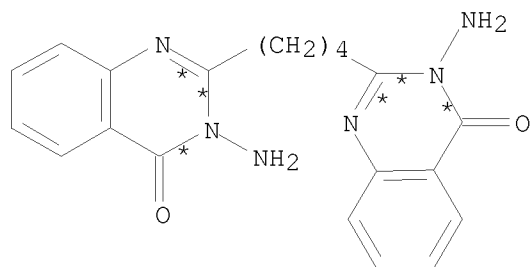
RX(14) RCT AF 352642-40-1  
RGT M 302-01-2 N2H4  
PRO AJ 623928-09-6  
SOL 71-36-3 BuOH  
CON SUBSTAGE(1) 6 - 8 hours, reflux  
SUBSTAGE(2) reflux -> 0 deg C

RX(15) OF 67 ...AH ==> AK...



AH

(15)  
→



AK  
YIELD 76%

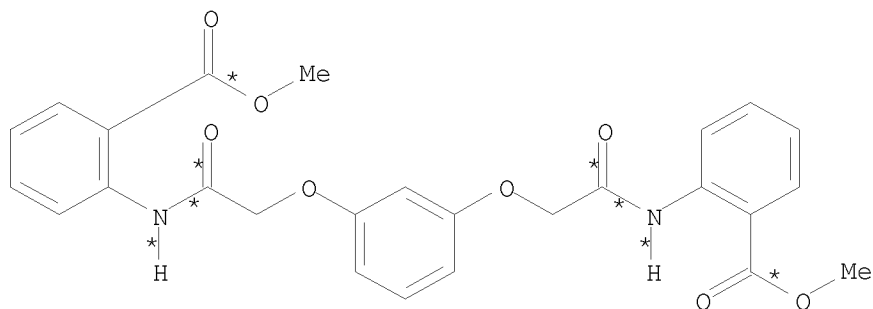
RX(15) RCT AH 68191-40-2  
RGT M 302-01-2 N2H4  
PRO AK 623928-10-9  
SOL 71-36-3 BuOH

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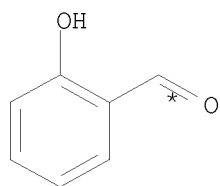
CON SUBSTAGE(1) 6 - 8 hours, reflux  
SUBSTAGE(2) reflux -> 0 deg C

RX(28) OF 67 COMPOSED OF RX(3), RX(4)

RX(28) I + 2 O ==> P

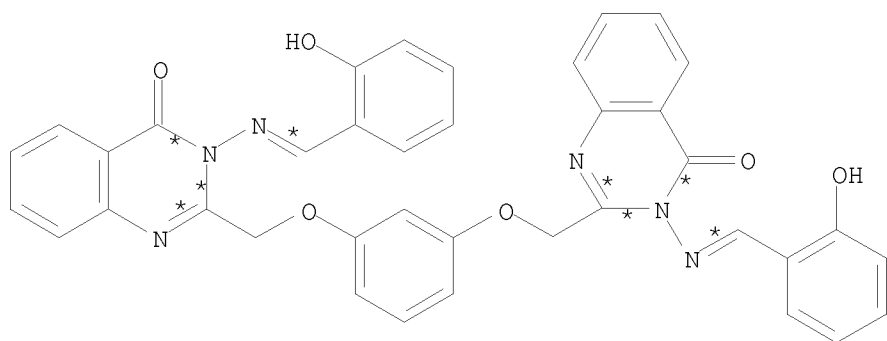


I



2 O

2  
STEPS  
→



P  
YIELD 60%

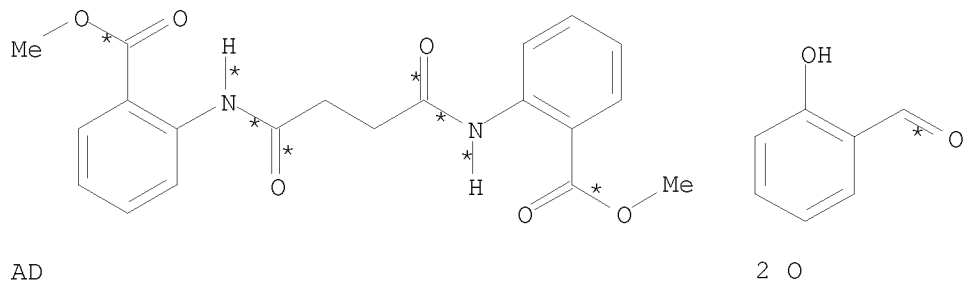
RX(3) RCT I 623928-01-8  
RGT M 302-01-2 N2H4  
PRO L 181770-29-6  
SOL 71-36-3 BuOH  
CON SUBSTAGE(1) 6 - 10 hours, reflux

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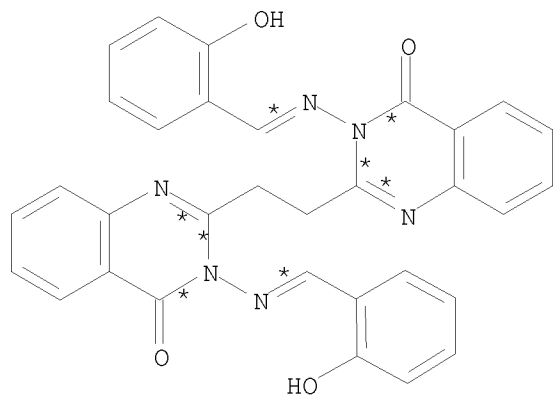
SUBSTAGE(2) reflux -> 0 deg C

RX(4) RCT L 181770-29-6, O 90-02-8  
PRO P 623928-04-1  
SOL 64-19-7 AcOH  
CON 3 hours

RX(36) OF 67 COMPOSED OF RX(13), RX(16)  
RX(36) AD + 2 O ==> AL



2  
STEPS  
→



AL  
YIELD 61%

RX(13) RCT AD 501938-94-9  
RGT M 302-01-2 N2H4  
PRO AI 623928-08-5  
SOL 71-36-3 BuOH  
CON SUBSTAGE(1) 6 - 8 hours, reflux  
SUBSTAGE(2) reflux -> 0 deg C

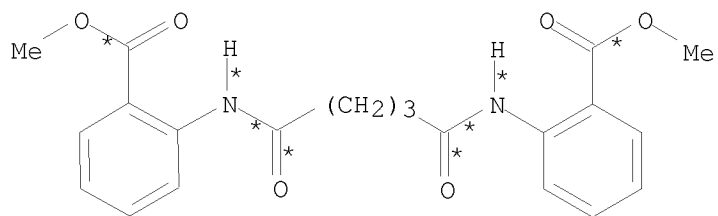
RX(16) RCT AI 623928-08-5, O 90-02-8  
PRO AL 623928-11-0  
SOL 64-19-7 AcOH

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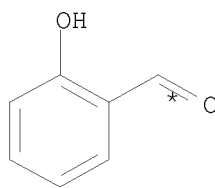
CON 1 hour, reflux

RX(38) OF 67 COMPOSED OF RX(14), RX(17)

RX(38) AF + 2 O ==> AM

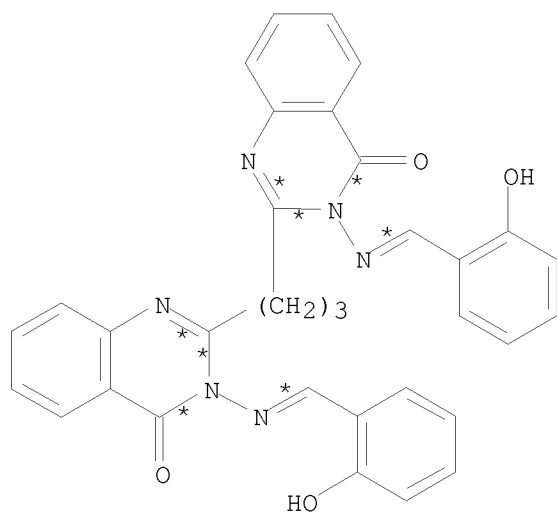


AF



2 O

2  
STEPS  
→



AM

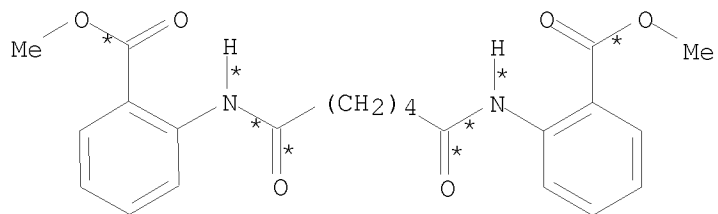
YIELD 64%

RX(14) RCT AF 352642-40-1  
RGT M 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO AJ 623928-09-6  
SOL 71-36-3 BuOH  
CON SUBSTAGE(1) 6 - 8 hours, reflux  
SUBSTAGE(2) reflux -> 0 deg C

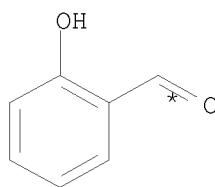
RX(17) RCT AJ 623928-09-6, O 90-02-8  
PRO AM 623928-12-1  
SOL 64-19-7 AcOH  
CON 1 hour, reflux

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RX(40) OF 67 COMPOSED OF RX(15), RX(18)  
RX(40) AH + 2 O ==> AN

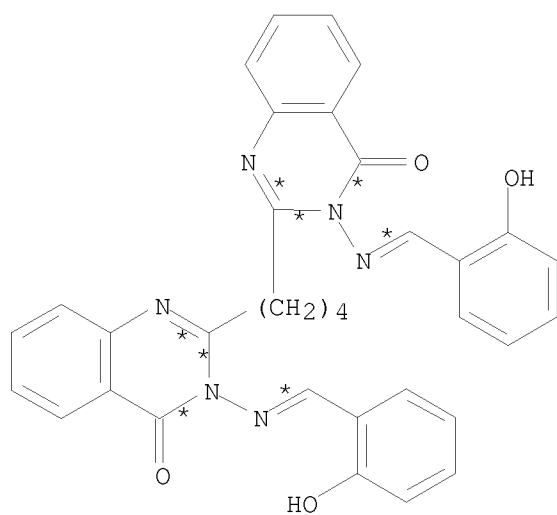


AH



2 O

2  
STEPS  
→



AN  
YIELD 60%

RX(15) RCT AH 68191-40-2  
RGT M 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO AK 623928-10-9  
SOL 71-36-3 BuOH  
CON SUBSTAGE(1) 6 - 8 hours, reflux  
SUBSTAGE(2) reflux -> 0 deg C

RX(18) RCT AK 623928-10-9, O 90-02-8  
PRO AN 623928-13-2  
SOL 64-19-7 AcOH  
CON 1 hour, reflux



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 83 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 139:337939 CASREACT

TITLE: Yb(OTf)<sub>3</sub>-catalyzed one-pot synthesis of quinazolin-4(3H)-ones from anthranilic acid, amines and ortho esters (or formic acid) in solvent-free conditions

AUTHOR(S): Wang, Limin; Xia, Jianjun; Qin, Fang; Qian, Changtao; Sun, Jie

CORPORATE SOURCE: Institute of Fine Chemicals, East China University of Science and Technology, Shanghai, 200237, Peop. Rep. China

SOURCE: Synthesis (2003), (8), 1241-1247  
CODEN: SYNTBF; ISSN: 0039-7881

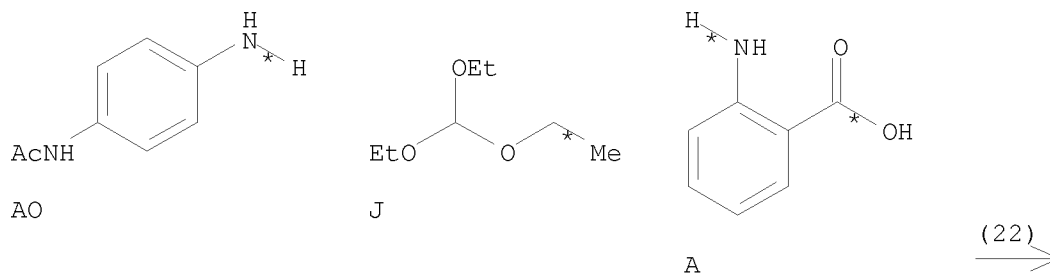
PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

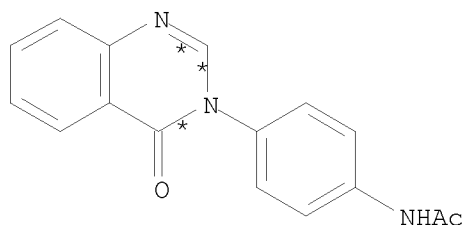
LANGUAGE: English

AB An efficient synthesis of an array of 4(3H)-quinazolinone derivs. from anthranilic acid, ortho esters (or formic acid) and amines using Yb(OTf)<sub>3</sub> in one-pot under solvent-free conditions is described. Compared with the classical reaction conditions, this new synthetic method has the advantage of excellent yields (75-99%), shorter reaction time (few minutes) and re-usability of the catalyst. Compds. thus prepared included 3-phenyl-4(3H)-quinazolinone, 3-(2-methylphenyl)-4(3H)-quinazolinone, 3-(4-methylphenyl)-4(3H)-quinazolinone, 3-(3,4-dimethylphenyl)-4(3H)-quinazolinone, 3-(4-ethylphenyl)-4(3H)-quinazolinone, 3-(4-methoxyphenyl)-4(3H)-quinazolinone, 3-(4-Chlorophenyl)-4(3H)-quinazolinone, 3-(4-fluorophenyl)-4(3H)-quinazolinone, 3-(4-nitrophenyl)-4(3H)-quinazolinone, etc. The lanthanide-mediated formation of an imidic ester intermediate was discussed.

RX(22) OF 24 AO + J + A ==> AP



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AP  
YIELD 97%

RX(22) RCT AO 122-80-5, J 122-51-0, A 118-92-3

STAGE(1)

CAT 54761-04-5 Methanesulfonic acid, 1,1,1-trifluoro-,  
ytterbium(3+) salt (3:1)  
CON 2 minutes, 60 deg C

STAGE(2)

SOL 7732-18-5 Water

PRO AP 24122-35-8

REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 84 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 139:181529 CASREACT

TITLE: Dyeing behaviour of some novel acid dyes on silk, wool  
and nylon fabrics

AUTHOR(S): Rana, U. N.; Patel, K. C.; Patel, S. K.

CORPORATE SOURCE: Department of Chemistry, South Gujarat University,  
Surat, 395 007, India

SOURCE: Ultra Scientist of Physical Sciences (2002), 14(3),  
353-360

CODEN: USPSE5

PUBLISHER: Ultra Scientist of Physical Sciences

DOCUMENT TYPE: Journal

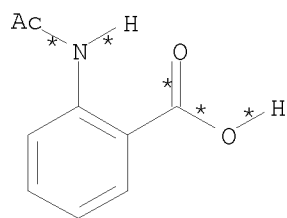
LANGUAGE: English

AB Ten azo dyes have been prepared by coupling diazotized  
2-methyl-3-(2-chlorophenyl)-6-amino-4-oxoquinazoline with various coupling  
acid components and their dyeing performance on silk, wool, and nylon has  
been assessed. All the dyes gave a wide range of brown shades with very  
good depth and levelness. The purity of all dyes has been checked by TLC.  
The IR spectra showed all characteristic bands and a representative dye  
PMR spectrum showed all the characteristic signals. The percentage  
dye-bath exhaustion and fixation on different fibers was reasonably  
moderate to very good.

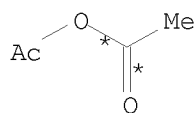
RX(15) OF 60 COMPOSED OF RX(11), RX(12)

RX(15) AA + AB + AD ==> AE

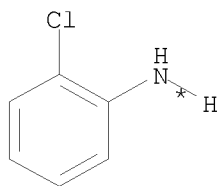
10/ 562,112



AA

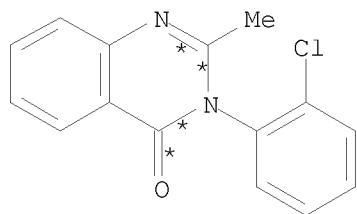


AB



AD

2  
STEPS  
→



AE  
YIELD 85%

RX(11) RCT AA 89-52-1, AB 108-24-7  
PRO AC 525-76-8  
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

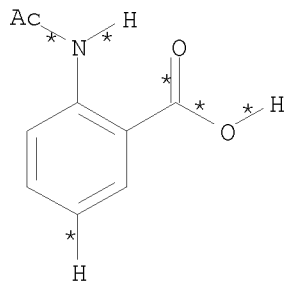
STAGE(1)  
CON 8 - 10 hours, 150 - 180 deg C

STAGE(2)  
RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water

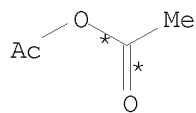
PRO AE 340-57-8

RX(28) OF 60 COMPOSED OF RX(11), RX(12), RX(13)

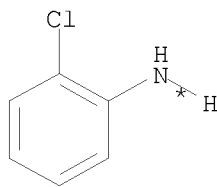
RX(28) AA + AB + AD ==> AF



AA



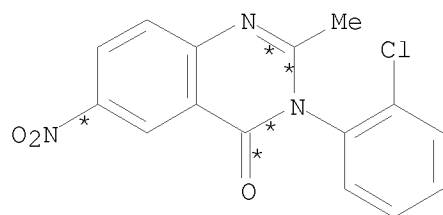
AB



AD

3  
STEPS  
→

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AF  
YIELD 90%

RX(11) RCT AA 89-52-1, AB 108-24-7  
PRO AC 525-76-8  
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

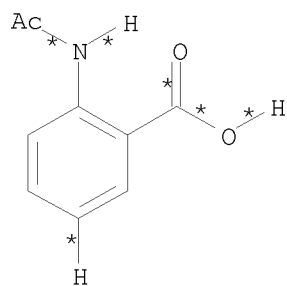
STAGE(1)  
CON 8 - 10 hours, 150 - 180 deg C

STAGE(2)  
RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water

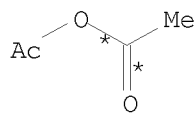
PRO AE 340-57-8

RX(13) RCT AE 340-57-8  
RGT AG 7697-37-2 HNO3  
PRO AF 1038-70-6  
SOL 7664-93-9 H2SO4  
CON SUBSTAGE(1) <75 deg C  
SUBSTAGE(2) overnight

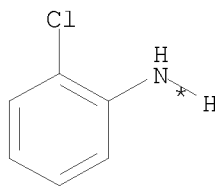
RX(30) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14)  
RX(30) AA + AB + AD ==> A



AA



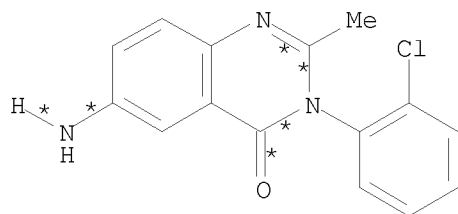
AB



AD

4  
STEPS  
➤

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A  
YIELD 85%

RX(11) RCT AA 89-52-1, AB 108-24-7  
PRO AC 525-76-8  
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

STAGE(1)  
CON 8 - 10 hours, 150 - 180 deg C

STAGE(2)  
RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO AE 340-57-8

RX(13) RCT AE 340-57-8  
RGT AG 7697-37-2 HNO3  
PRO AF 1038-70-6  
SOL 7664-93-9 H2SO4  
CON SUBSTAGE(1) <75 deg C  
SUBSTAGE(2) overnight

RX(14) RCT AF 1038-70-6

STAGE(1)  
RGT AI 1313-82-2 Na2S  
SOL 7732-18-5 Water  
CON 2 hours, reflux

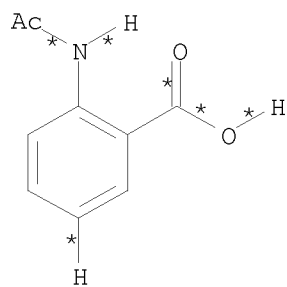
STAGE(2)  
RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 20 minutes, reflux

STAGE(3)  
RGT G 497-19-8 Na2CO3

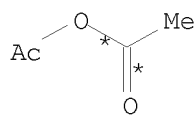
PRO A 963-35-9

RX(51) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(1)  
RX(51) AA + AB + AD + B ==> C

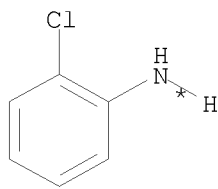
10/ 562,112



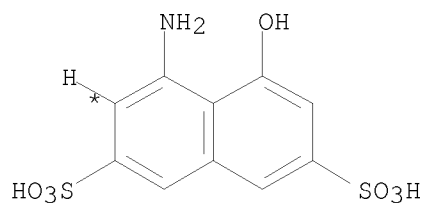
AA



AB

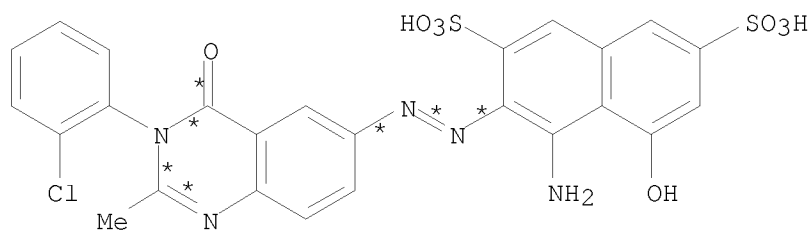


AD



B

5  
STEPS  
→



● 2 Na

C  
YIELD 85%

RX(11) RCT AA 89-52-1, AB 108-24-7  
PRO AC 525-76-8  
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

STAGE(1)

CON 8 - 10 hours, 150 - 180 deg C

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

10/ 562,112

PRO AE 340-57-8

RX(13) RCT AE 340-57-8  
RGT AG 7697-37-2 HNO3  
PRO AF 1038-70-6  
SOL 7664-93-9 H2SO4  
CON SUBSTAGE(1) <75 deg C  
SUBSTAGE(2) overnight

RX(14) RCT AF 1038-70-6

STAGE(1)  
RGT AI 1313-82-2 Na2S  
SOL 7732-18-5 Water  
CON 2 hours, reflux

STAGE(2)  
RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 20 minutes, reflux

STAGE(3)  
RGT G 497-19-8 Na2CO3

PRO A 963-35-9

RX(1) RCT A 963-35-9

STAGE(1)  
RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) room temperature -> 70 deg C  
SUBSTAGE(2) 70 deg C -> 0 deg C

STAGE(2)  
RGT E 7632-00-0 NaNO2  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 5 minutes, 0 - 5 deg C  
SUBSTAGE(2) 1 hour, 0 - 5 deg C

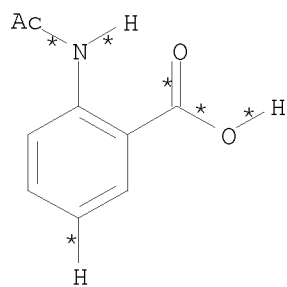
STAGE(3)  
RGT F 5329-14-6 Sulfamic acid

STAGE(4)  
RCT B 90-20-0  
RGT G 497-19-8 Na2CO3  
CON SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8  
SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

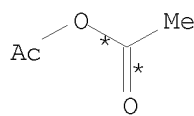
PRO C 577040-28-9

RX(52) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(2)  
RX(52) AA + AB + AD + I ==> J

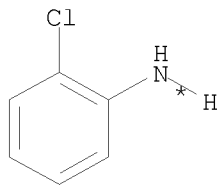
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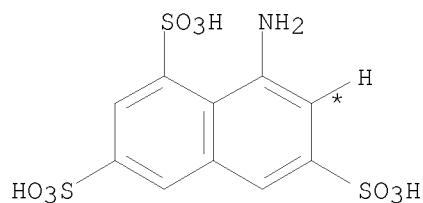
AA



AB

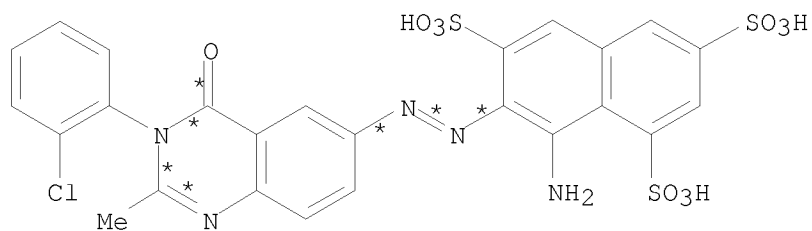


AD



I

5  
STEPS  
→



● 3 Na

J  
YIELD 80%

RX(11) RCT AA 89-52-1, AB 108-24-7  
PRO AC 525-76-8  
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

STAGE(1)

CON 8 - 10 hours, 150 - 180 deg C

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water



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PRO AE 340-57-8

RX(13) RCT AE 340-57-8  
RGT AG 7697-37-2 HNO3  
PRO AF 1038-70-6  
SOL 7664-93-9 H2SO4  
CON SUBSTAGE(1) <75 deg C  
SUBSTAGE(2) overnight

RX(14) RCT AF 1038-70-6

STAGE(1)  
RGT AI 1313-82-2 Na2S  
SOL 7732-18-5 Water  
CON 2 hours, reflux

STAGE(2)  
RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 20 minutes, reflux

STAGE(3)  
RGT G 497-19-8 Na2CO3

PRO A 963-35-9

RX(2) RCT A 963-35-9

STAGE(1)  
RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) room temperature -> 70 deg C  
SUBSTAGE(2) 70 deg C -> 0 deg C

STAGE(2)  
RGT E 7632-00-0 NaNO2  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 5 minutes, 0 - 5 deg C  
SUBSTAGE(2) 1 hour, 0 - 5 deg C

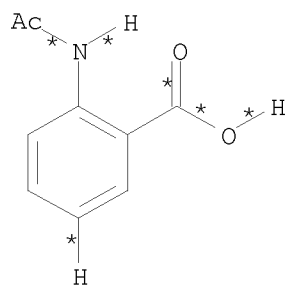
STAGE(3)  
RGT F 5329-14-6 Sulfamic acid

STAGE(4)  
RCT I 117-42-0  
RGT G 497-19-8 Na2CO3  
CON SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8  
SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

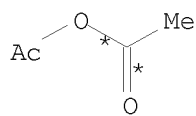
PRO J 577040-29-0

RX(53) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(3)  
RX(53) AA + AB + AD + K ==> L

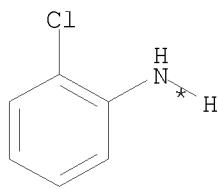
10/ 562,112



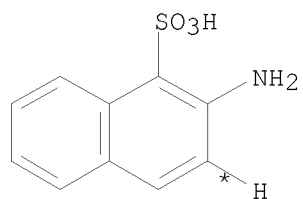
AA



AB

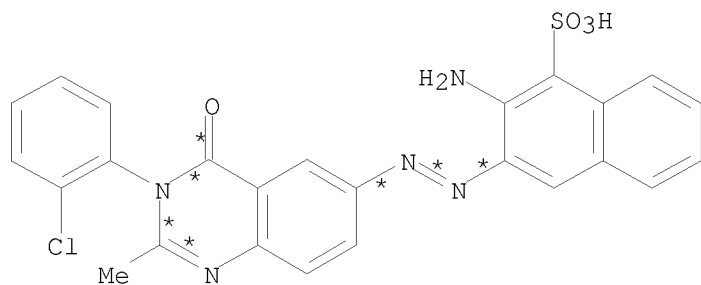


AD



K

5  
STEPS  
→



● Na

L  
YIELD 78%

RX(11) RCT AA 89-52-1, AB 108-24-7  
PRO AC 525-76-8  
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

STAGE(1)  
CON 8 - 10 hours, 150 - 180 deg C

STAGE(2)

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RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO AE 340-57-8

RX(13) RCT AE 340-57-8  
RGT AG 7697-37-2 HNO3  
PRO AF 1038-70-6  
SOL 7664-93-9 H2SO4  
CON SUBSTAGE(1) <75 deg C  
SUBSTAGE(2) overnight

RX(14) RCT AF 1038-70-6

STAGE(1)  
RGT AI 1313-82-2 Na2S  
SOL 7732-18-5 Water  
CON 2 hours, reflux

STAGE(2)  
RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 20 minutes, reflux

STAGE(3)  
RGT G 497-19-8 Na2CO3

PRO A 963-35-9

RX(3) RCT A 963-35-9

STAGE(1)  
RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) room temperature -> 70 deg C  
SUBSTAGE(2) 70 deg C -> 0 deg C

STAGE(2)  
RGT E 7632-00-0 NaNO2  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 5 minutes, 0 - 5 deg C  
SUBSTAGE(2) 1 hour, 0 - 5 deg C

STAGE(3)  
RGT F 5329-14-6 Sulfamic acid

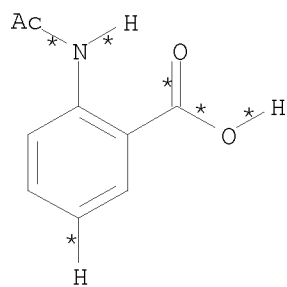
STAGE(4)  
RCT K 81-16-3  
RGT G 497-19-8 Na2CO3  
CON SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8  
SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

PRO L 577040-30-3

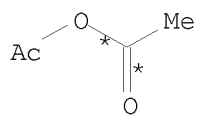
RX(54) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(4)

RX(54) AA + AB + AD + M ==> N

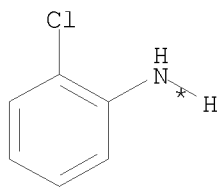
10/ 562,112



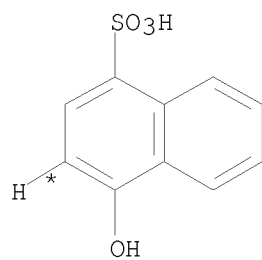
AA



AB

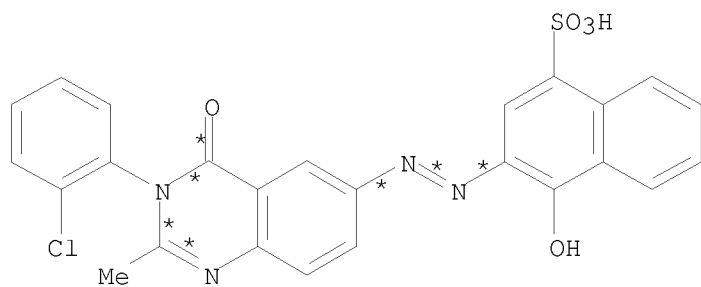


AD



M

5  
STEPS  
→



● Na

N  
YIELD 72%

RX(11) RCT AA 89-52-1, AB 108-24-7  
PRO AC 525-76-8  
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

STAGE(1)  
CON 8 - 10 hours, 150 - 180 deg C

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```

    STAGE(2)
      RGT  D 7647-01-0 HCl
      SOL  7732-18-5 Water

PRO  AE 340-57-8

RX(13)  RCT  AE 340-57-8
        RGT  AG 7697-37-2 HNO3
        PRO  AF 1038-70-6
        SOL  7664-93-9 H2SO4
        CON  SUBSTAGE(1) <75 deg C
              SUBSTAGE(2) overnight

RX(14)  RCT  AF 1038-70-6

    STAGE(1)
      RGT  AI 1313-82-2 Na2S
      SOL  7732-18-5 Water
      CON  2 hours, reflux

    STAGE(2)
      RGT  D 7647-01-0 HCl
      SOL  7732-18-5 Water
      CON  20 minutes, reflux

    STAGE(3)
      RGT  G 497-19-8 Na2CO3

PRO  A 963-35-9

RX(4)  RCT  A 963-35-9

    STAGE(1)
      RGT  D 7647-01-0 HCl
      SOL  7732-18-5 Water
      CON  SUBSTAGE(1) room temperature -> 70 deg C
            SUBSTAGE(2) 70 deg C -> 0 deg C

    STAGE(2)
      RGT  E 7632-00-0 NaNO2
      SOL  7732-18-5 Water
      CON  SUBSTAGE(1) 5 minutes, 0 - 5 deg C
            SUBSTAGE(2) 1 hour, 0 - 5 deg C

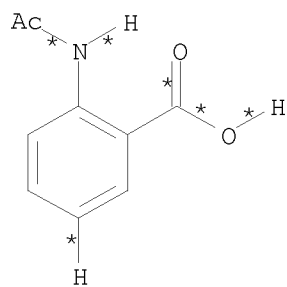
    STAGE(3)
      RGT  F 5329-14-6 Sulfamic acid

    STAGE(4)
      RCT  M 84-87-7
      RGT  G 497-19-8 Na2CO3
      CON  SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8
            SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

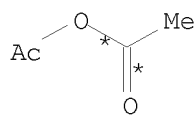
PRO  N 577040-31-4

RX(55) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(5)
RX(55)  AA  +  AB  +  AD  +  O  ==>  P
```

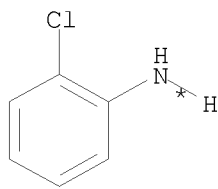
10/ 562,112



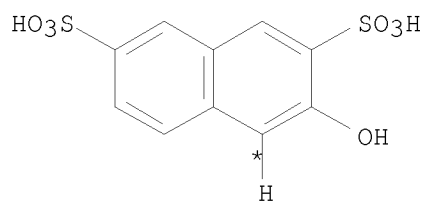
AA



AB

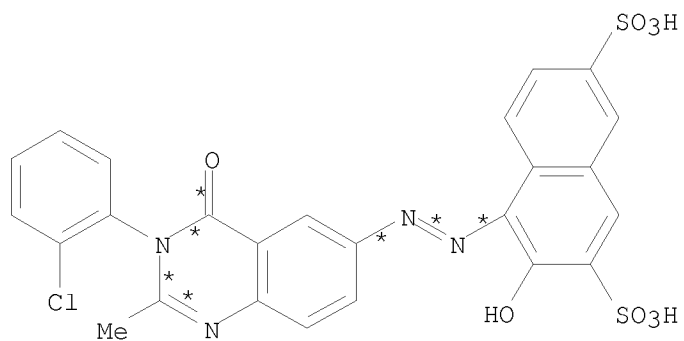


AD



O

5  
STEPS  
→



● 2 Na

P  
YIELD 82%

RX(11) RCT AA 89-52-1, AB 108-24-7  
PRO AC 525-76-8  
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

STAGE(1)  
CON 8 - 10 hours, 150 - 180 deg C

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```

    STAGE(2)
      RGT  D 7647-01-0 HCl
      SOL  7732-18-5 Water

PRO   AE 340-57-8

RX(13)  RCT  AE 340-57-8
        RGT  AG 7697-37-2 HNO3
        PRO  AF 1038-70-6
        SOL  7664-93-9 H2SO4
        CON  SUBSTAGE(1) <75 deg C
              SUBSTAGE(2) overnight

RX(14)  RCT  AF 1038-70-6

    STAGE(1)
      RGT  AI 1313-82-2 Na2S
      SOL  7732-18-5 Water
      CON  2 hours, reflux

    STAGE(2)
      RGT  D 7647-01-0 HCl
      SOL  7732-18-5 Water
      CON  20 minutes, reflux

    STAGE(3)
      RGT  G 497-19-8 Na2CO3

PRO   A 963-35-9

RX(5)  RCT  A 963-35-9

    STAGE(1)
      RGT  D 7647-01-0 HCl
      SOL  7732-18-5 Water
      CON  SUBSTAGE(1) room temperature -> 70 deg C
            SUBSTAGE(2) 70 deg C -> 0 deg C

    STAGE(2)
      RGT  E 7632-00-0 NaNO2
      SOL  7732-18-5 Water
      CON  SUBSTAGE(1) 5 minutes, 0 - 5 deg C
            SUBSTAGE(2) 1 hour, 0 - 5 deg C

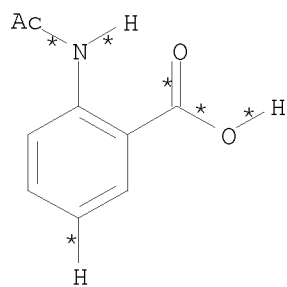
    STAGE(3)
      RGT  F 5329-14-6 Sulfamic acid

    STAGE(4)
      RCT  O 148-75-4
      RGT  G 497-19-8 Na2CO3
      CON  SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8
            SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

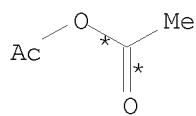
PRO   P 577040-32-5

RX(56) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(6)
RX(56)  AA  +  AB  +  AD  +  Q  ==>  R
```

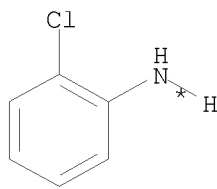
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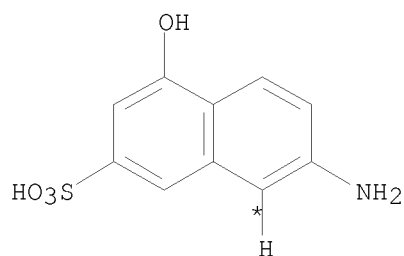
AA



AB

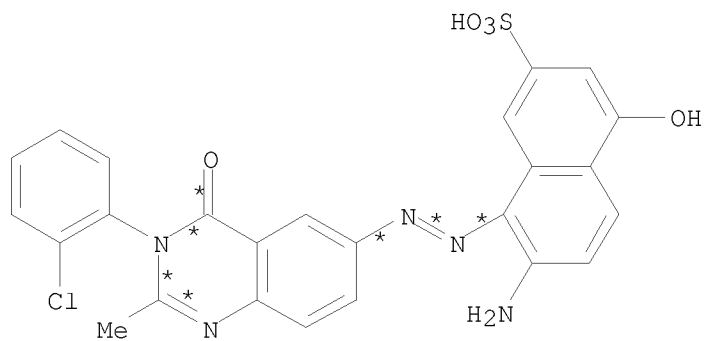


AD



Q

5  
STEPS  
→



● Na

R  
YIELD 87%

RX(11) RCT AA 89-52-1, AB 108-24-7  
PRO AC 525-76-8  
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2



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```

    STAGE(1)
      CON  8 - 10 hours, 150 - 180 deg C

    STAGE(2)
      RGT  D 7647-01-0 HCl
      SOL  7732-18-5 Water

    PRO  AE 340-57-8

RX(13)  RCT  AE 340-57-8
        RGT  AG 7697-37-2 HNO3
        PRO  AF 1038-70-6
        SOL  7664-93-9 H2SO4
        CON  SUBSTAGE(1) <75 deg C
              SUBSTAGE(2) overnight

RX(14)  RCT  AF 1038-70-6

    STAGE(1)
      RGT  AI 1313-82-2 Na2S
      SOL  7732-18-5 Water
      CON  2 hours, reflux

    STAGE(2)
      RGT  D 7647-01-0 HCl
      SOL  7732-18-5 Water
      CON  20 minutes, reflux

    STAGE(3)
      RGT  G 497-19-8 Na2CO3

    PRO  A 963-35-9

RX(6)   RCT  A 963-35-9

    STAGE(1)
      RGT  D 7647-01-0 HCl
      SOL  7732-18-5 Water
      CON  SUBSTAGE(1) room temperature -> 70 deg C
            SUBSTAGE(2) 70 deg C -> 0 deg C

    STAGE(2)
      RGT  E 7632-00-0 NaNO2
      SOL  7732-18-5 Water
      CON  SUBSTAGE(1) 5 minutes, 0 - 5 deg C
            SUBSTAGE(2) 1 hour, 0 - 5 deg C

    STAGE(3)
      RGT  F 5329-14-6 Sulfamic acid

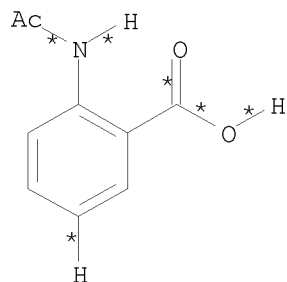
    STAGE(4)
      RCT  Q 87-02-5
      RGT  G 497-19-8 Na2CO3
      CON  SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8
            SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

    PRO  R 577040-33-6
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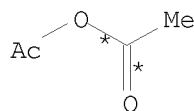
RX(57) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(7)

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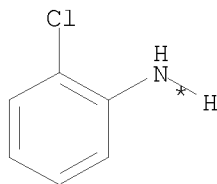
RX(57)      AA   +   AB   +   AD   +   S   ==>   T



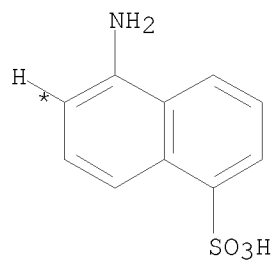
AA



AB

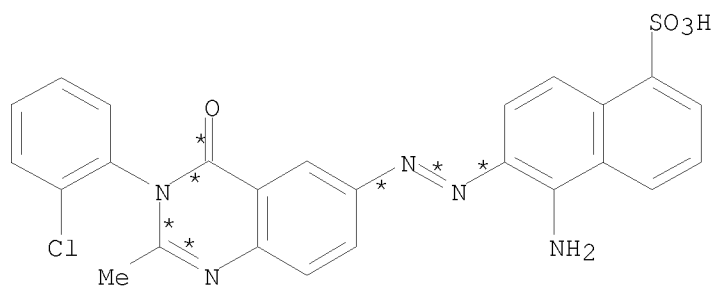


AD



S

5  
STEPS  
→



● Na

T  
YIELD 72%

RX(11)      RCT    AA 89-52-1, AB 108-24-7  
              PRO    AC 525-76-8  
              CON    30 minutes, reflux

RX(12)      RCT    AC 525-76-8, AD 95-51-2

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```

    STAGE(1)
      CON  8 - 10 hours, 150 - 180 deg C

    STAGE(2)
      RGT  D 7647-01-0 HCl
      SOL  7732-18-5 Water

    PRO  AE 340-57-8

RX(13)  RCT  AE 340-57-8
        RGT  AG 7697-37-2 HNO3
        PRO  AF 1038-70-6
        SOL  7664-93-9 H2SO4
        CON  SUBSTAGE(1) <75 deg C
              SUBSTAGE(2) overnight

RX(14)  RCT  AF 1038-70-6

    STAGE(1)
      RGT  AI 1313-82-2 Na2S
      SOL  7732-18-5 Water
      CON  2 hours, reflux

    STAGE(2)
      RGT  D 7647-01-0 HCl
      SOL  7732-18-5 Water
      CON  20 minutes, reflux

    STAGE(3)
      RGT  G 497-19-8 Na2CO3

    PRO  A 963-35-9

RX(7)   RCT  A 963-35-9

    STAGE(1)
      RGT  D 7647-01-0 HCl
      SOL  7732-18-5 Water
      CON  SUBSTAGE(1) room temperature -> 70 deg C
            SUBSTAGE(2) 70 deg C -> 0 deg C

    STAGE(2)
      RGT  E 7632-00-0 NaNO2
      SOL  7732-18-5 Water
      CON  SUBSTAGE(1) 5 minutes, 0 - 5 deg C
            SUBSTAGE(2) 1 hour, 0 - 5 deg C

    STAGE(3)
      RGT  F 5329-14-6 Sulfamic acid

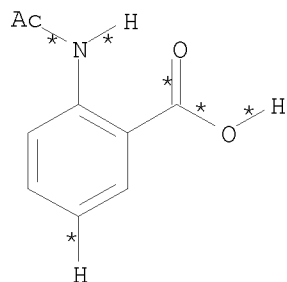
    STAGE(4)
      RCT  S 84-89-9
      RGT  G 497-19-8 Na2CO3
      CON  SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8
            SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

    PRO  T 577040-34-7

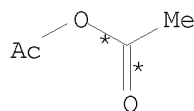
RX(58) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(8)
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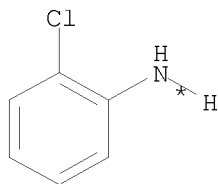
RX(58)      AA   +   AB   +   AD   +   U   ==>   V



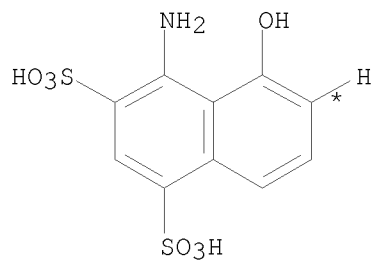
AA



AB

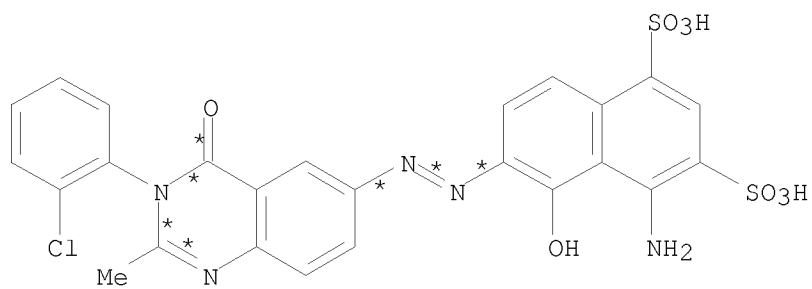


AD



U

5  
STEPS  
→



● 2 Na

V  
YIELD 76%

RX(11)      RCT    AA 89-52-1, AB 108-24-7  
              PRO    AC 525-76-8  
              CON    30 minutes, reflux

RX(12)      RCT    AC 525-76-8, AD 95-51-2

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```

    STAGE(1)
      CON  8 - 10 hours, 150 - 180 deg C

    STAGE(2)
      RGT  D 7647-01-0 HCl
      SOL  7732-18-5 Water

    PRO  AE 340-57-8

RX(13)  RCT  AE 340-57-8
        RGT  AG 7697-37-2 HNO3
        PRO  AF 1038-70-6
        SOL  7664-93-9 H2SO4
        CON  SUBSTAGE(1) <75 deg C
              SUBSTAGE(2) overnight

RX(14)  RCT  AF 1038-70-6

    STAGE(1)
      RGT  AI 1313-82-2 Na2S
      SOL  7732-18-5 Water
      CON  2 hours, reflux

    STAGE(2)
      RGT  D 7647-01-0 HCl
      SOL  7732-18-5 Water
      CON  20 minutes, reflux

    STAGE(3)
      RGT  G 497-19-8 Na2CO3

    PRO  A 963-35-9

RX(8)   RCT  A 963-35-9

    STAGE(1)
      RGT  D 7647-01-0 HCl
      SOL  7732-18-5 Water
      CON  SUBSTAGE(1) room temperature -> 70 deg C
            SUBSTAGE(2) 70 deg C -> 0 deg C

    STAGE(2)
      RGT  E 7632-00-0 NaNO2
      SOL  7732-18-5 Water
      CON  SUBSTAGE(1) 5 minutes, 0 - 5 deg C
            SUBSTAGE(2) 1 hour, 0 - 5 deg C

    STAGE(3)
      RGT  F 5329-14-6 Sulfamic acid

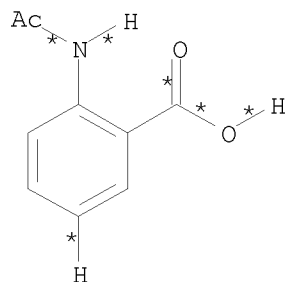
    STAGE(4)
      RCT  U 82-47-3
      RGT  G 497-19-8 Na2CO3
      CON  SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8
            SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

    PRO  V 577040-35-8

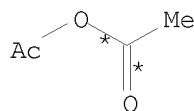
RX(59) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(9)
```

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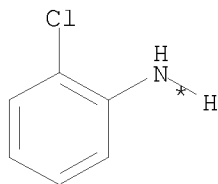
RX(59)      AA   +   AB   +   AD   +   W   ==>   X



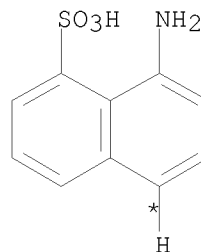
AA



AB

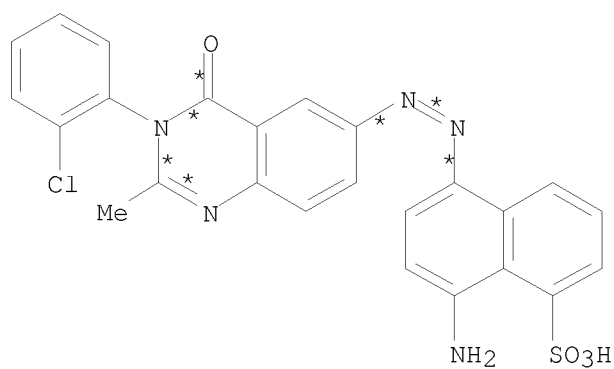


AD



W

5  
STEPS  
→



● Na

X  
YIELD 79%

RX(11)      RCT    AA 89-52-1, AB 108-24-7  
              PRO    AC 525-76-8  
              CON    30 minutes, reflux

RX(12)      RCT    AC 525-76-8, AD 95-51-2

STAGE(1)  
      CON    8 - 10 hours, 150 - 180 deg C

STAGE(2)  
      RGT    D 7647-01-0 HCl  
      SOL    7732-18-5 Water

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PRO AE 340-57-8

RX(13) RCT AE 340-57-8  
RGT AG 7697-37-2 HNO3  
PRO AF 1038-70-6  
SOL 7664-93-9 H2SO4  
CON SUBSTAGE(1) <75 deg C  
SUBSTAGE(2) overnight

RX(14) RCT AF 1038-70-6

STAGE(1)  
RGT AI 1313-82-2 Na2S  
SOL 7732-18-5 Water  
CON 2 hours, reflux

STAGE(2)  
RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 20 minutes, reflux

STAGE(3)  
RGT G 497-19-8 Na2CO3

PRO A 963-35-9

RX(9) RCT A 963-35-9

STAGE(1)  
RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) room temperature -> 70 deg C  
SUBSTAGE(2) 70 deg C -> 0 deg C

STAGE(2)  
RGT E 7632-00-0 NaNO2  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 5 minutes, 0 - 5 deg C  
SUBSTAGE(2) 1 hour, 0 - 5 deg C

STAGE(3)  
RGT F 5329-14-6 Sulfamic acid

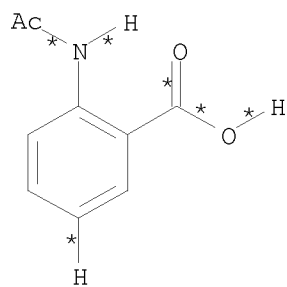
STAGE(4)  
RCT W 82-75-7  
RGT G 497-19-8 Na2CO3  
CON SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8  
SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

PRO X 577040-36-9

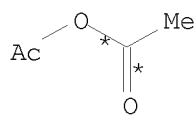
RX(60) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(10)

RX(60) AA + AB + AD + Y ==> Z

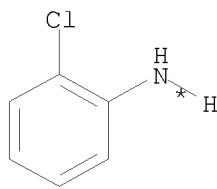
10/ 562,112



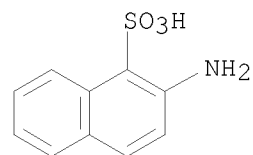
AA



AB



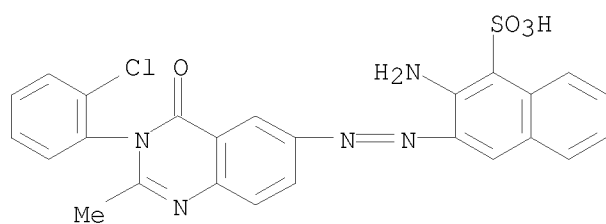
AD



D1-SO<sub>3</sub>H

Y

5  
STEPS  
→



D1-SO<sub>3</sub>H

● 2 Na

Z  
YIELD 82%

RX(11) RCT AA 89-52-1, AB 108-24-7  
PRO AC 525-76-8  
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

STAGE(1)  
CON 8 - 10 hours, 150 - 180 deg C

STAGE(2)  
RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO AE 340-57-8

RX(13) RCT AE 340-57-8  
RGT AG 7697-37-2 HNO<sub>3</sub>



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PRO AF 1038-70-6  
SOL 7664-93-9 H2SO4  
CON SUBSTAGE(1) <75 deg C  
SUBSTAGE(2) overnight

RX(14) RCT AF 1038-70-6

STAGE(1)  
RGT AI 1313-82-2 Na2S  
SOL 7732-18-5 Water  
CON 2 hours, reflux

STAGE(2)  
RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 20 minutes, reflux

STAGE(3)  
RGT G 497-19-8 Na2CO3

PRO A 963-35-9

RX(10) RCT A 963-35-9

STAGE(1)  
RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) room temperature -> 70 deg C  
SUBSTAGE(2) 70 deg C -> 0 deg C

STAGE(2)  
RGT E 7632-00-0 NaNO2  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 5 minutes, 0 - 5 deg C  
SUBSTAGE(2) 1 hour, 0 - 5 deg C

STAGE(3)  
RGT F 5329-14-6 Sulfamic acid

STAGE(4)  
RCT Y 171570-11-9  
RGT G 497-19-8 Na2CO3  
CON SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8  
SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

PRO Z 577969-58-5

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 85 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 139:101143 CASREACT

TITLE: Preparation of quinazolinone derivatives having  
poly(adenosine 5'-diphosphoribose) polymerase  
inhibitory activity

INVENTOR(S): Ishida, Junya; Hattori, Kouji; Kido, Yoshiyuki

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan

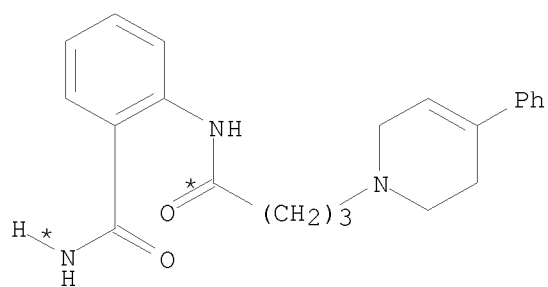
SOURCE: PCT Int. Appl., 35 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003055865	A1	20030710	WO 2002-JP13286	20021219
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2471348	A1	20030710	CA 2002-2471348	20021219
AU 2002353537	A1	20030715	AU 2002-353537	20021219
EP 1458688	A1	20040922	EP 2002-788856	20021219
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			
JP 2005515216	T	20050526	JP 2003-556396	20021219
US 20050043333	A1	20050224	US 2004-499348	20040617
PRIORITY APPLN. INFO.:			AU 2001-9756	20011224
			WO 2002-JP13286	20021219
OTHER SOURCE(S):		MARPAT 139:101143		
GI				

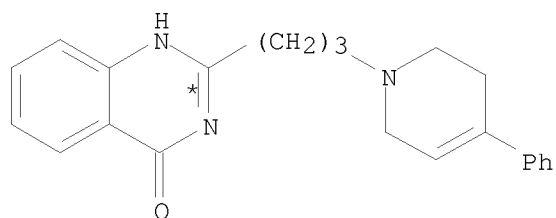
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Quinazolinone derivs. I [R1 = substituted cyclic amino, (un)substituted amino; R2 = substituent - halogen, lower alkyl, lower alkoxy; n = integer from 0 to 4; L1 = (1) cyclo (lower) alkylene, (2) cyclo (lower) alkenylene, (3) diradical of (un)saturated monocyclic group with one or more nitrogen atom(s), which is obtained after removal of one hydrogen atom from said monocyclic group, or (4) -N(R3)-L2-; R3 = H, lower alkyl; L2 = lower alkylene or lower alkenylene], or its prodrug, or a salt thereof having poly(adenosine 5'-diphospho-ribose) polymerase (PARP) inhibitory activity and their preparation from benzamides II are described. Thus, III was prepared via cyclization of benzamide IV in dioxane with aqueous NaOH. PARP inhibitory activity of I [] was determined (IC50 = <0.5  $\mu$ M).

RX(1) OF 5 A ==> B



A

(1)  $\longrightarrow$ 

B

YIELD 70%

RX(1) RCT A 437998-41-9

STAGE(1)

SOL 123-91-1 Dioxane

CON room temperature

STAGE(2)

RGT C 1310-73-2 NaOH

SOL 7732-18-5 Water

CON 15 hours, room temperature

PRO B 437995-37-4

NTE key step

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 86 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 139:69214 CASREACT

TITLE: Improved synthesis of  
3-(2-ethylphenyl)-2-methyl-4(3H)-quinazolinone  
hydrochloride

AUTHOR(S): Yu, Hong-Xia; Guo, Feng; Xu, Xiong-li

CORPORATE SOURCE: Department Pharmacy, Wuhan Inst. Chem. Technol.,  
Wuhan, 430073, Peop. Rep. China

SOURCE: Wuhan Huagong Xueyuan Xuebao (2002), 24(4), 13-14

CODEN: WXUXEY; ISSN: 1004-4736

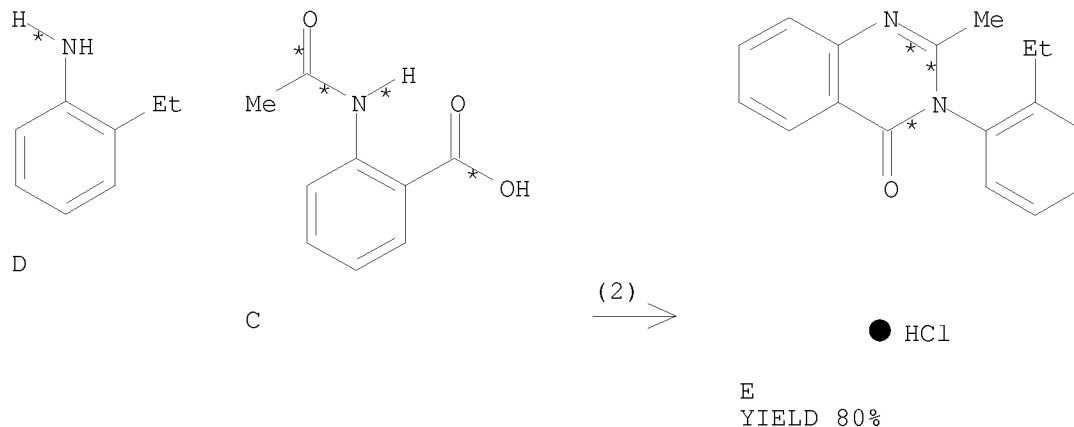
PUBLISHER: Wuhan Huagong Xueyuan Xuebao Bianjibu

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB Refluxing 2-acetylaminobenzoic acid with 2-ethylaniline in toluene in the presence of POCl<sub>3</sub> for 3 h gave 80% the title compound

RX(2) OF 3 ...D + C ==&gt; E



RX(2) RCT D 578-54-1, C 89-52-1  
 RGT F 10025-87-3 POCl<sub>3</sub>  
 PRO E 97979-65-2  
 SOL 108-88-3 PhMe  
 CON 3 hours, reflux

L3 ANSWER 87 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 139:22171 CASREACT

TITLE: Synthesis of some new substituted  
 $\beta$ -(quinazolin-2-yl) acrylic acid derivatives of  
 expected biological activity

AUTHOR(S): Nassar, S. A.; Aly, A. A.

CORPORATE SOURCE: Chemistry Department, Faculty of Science, Benha  
 Branch, Zagazig University, Benha, Egypt

SOURCE: Egyptian Journal of Chemistry (2002), 45(1), 205-217  
 CODEN: EGJCA3; ISSN: 0449-2285

PUBLISHER: National Information and Documentation Centre

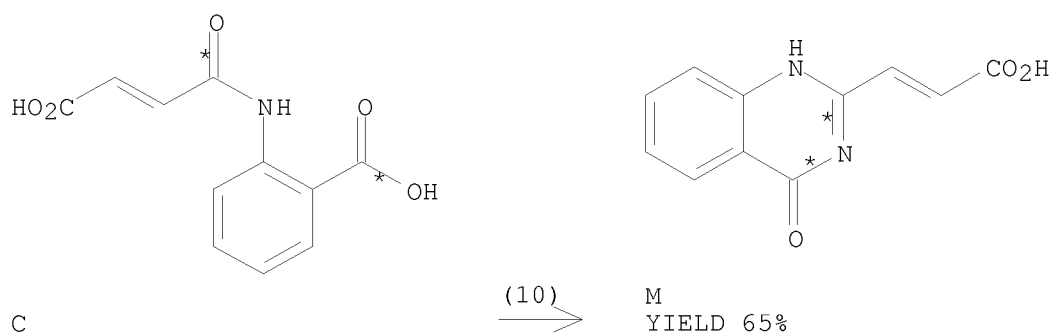
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Some new substituted  $\beta$ -(quinazolin-2-yl) acrylic acid derivs. were synthesized from the reaction of 2-(2'-carboxyethenyl)-4H-3,1-benzoxazin-4-one with nitrogen nucleophiles. The structures of the synthesized compds. were confirmed by IR, NMR, and mass spectral study. The products were screened for their antimicrobial activity. Most of the compds. exhibited moderate activity.

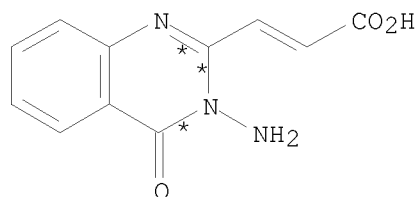
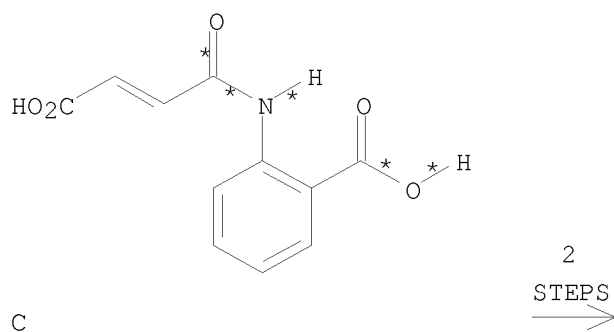
10/ 562,112

RX(10) OF 101 ...C ==> M...



RX(10) RCT C 68040-76-6  
RGT Z 631-61-8 NH4OAc  
PRO M 5584-96-3  
CON 1 hour, 170 deg C

RX(38) OF 101 COMPOSED OF RX(2), RX(3)  
RX(38) C ==> E



E  
YIELD 70%

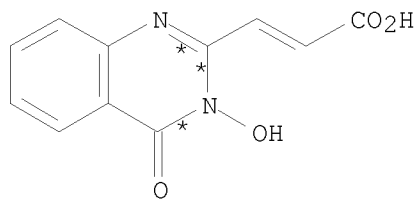
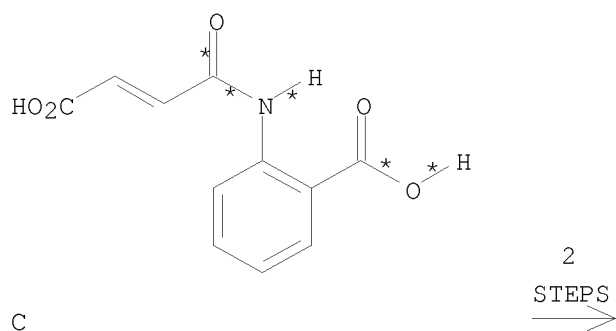
RX(2) RCT C 68040-76-6  
PRO D 107855-44-7  
CON 1 hour

RX(3) RCT D 107855-44-7

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RGT F 7803-57-8 N2H4-H2O  
PRO E 536741-94-3  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(39) OF 101 COMPOSED OF RX(2), RX(4)  
RX(39) C ==> H



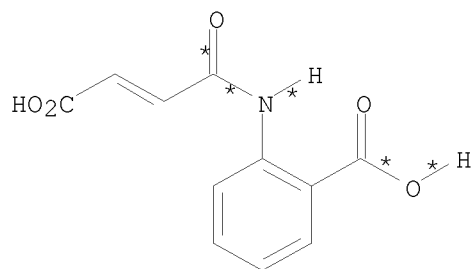
YIELD 75%

RX(2) RCT C 68040-76-6  
PRO D 107855-44-7  
CON 1 hour

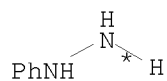
RX(4) RCT D 107855-44-7  
RGT I 5470-11-1 H2NOH-HCl, J 110-86-1 Pyridine  
PRO H 37833-86-6  
CON 4 hours, reflux

RX(40) OF 101 COMPOSED OF RX(2), RX(5)  
RX(40) C + K ==> L

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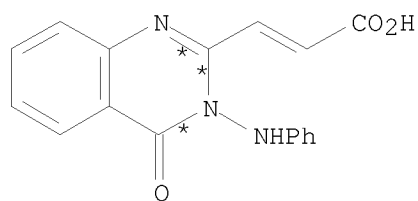


C



K

2  
STEPS  
→

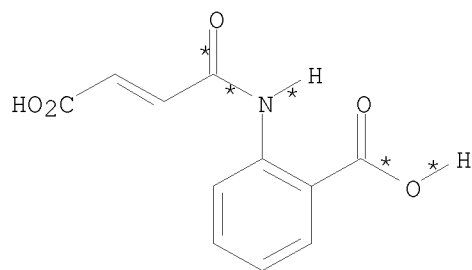


L  
YIELD 68%

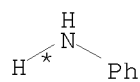
RX(2) RCT C 68040-76-6  
PRO D 107855-44-7  
CON 1 hour

RX(5) RCT D 107855-44-7, K 100-63-0  
RGT F 7803-57-8 N2H4-H2O  
PRO L 5958-13-4  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(41) OF 101 COMPOSED OF RX(2), RX(16)  
RX(41) C + AJ ==> AK



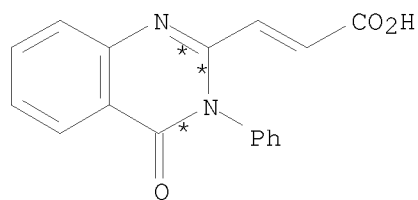
C



AJ

2  
STEPS  
→

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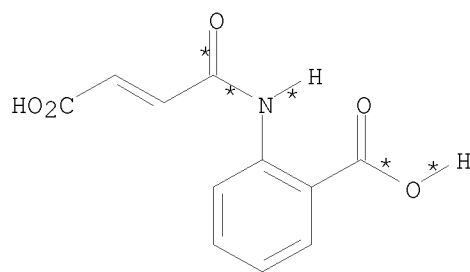
AK  
YIELD 74%

RX(2) RCT C 68040-76-6  
PRO D 107855-44-7  
CON 1 hour

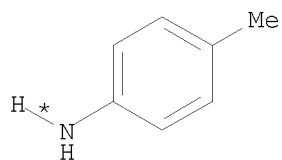
RX(16) RCT D 107855-44-7, AJ 62-53-3  
PRO AK 536742-04-8  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(42) OF 101 COMPOSED OF RX(2), RX(17)

RX(42) C + AL ==> AM

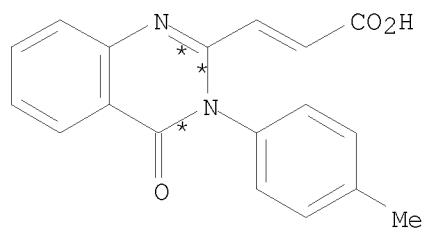


C



AL

2  
STEPS  
→



AM  
YIELD 70%

RX(2) RCT C 68040-76-6  
PRO D 107855-44-7

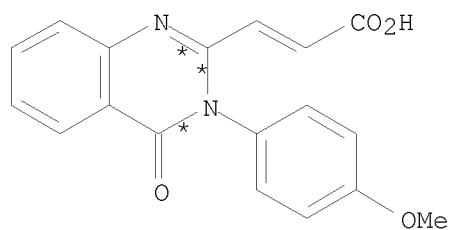
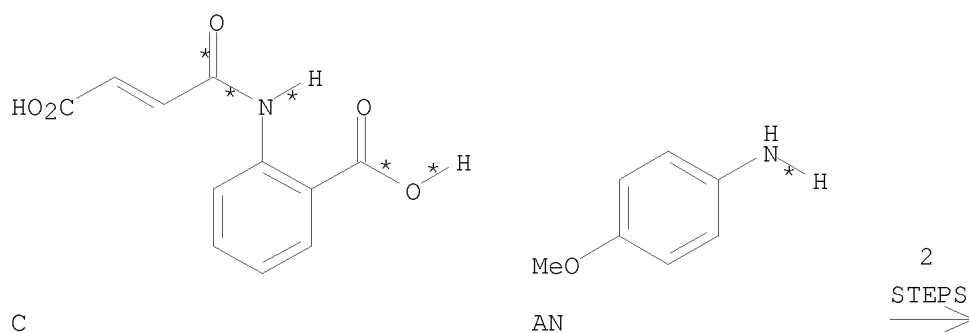


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CON 1 hour

RX(17) RCT D 107855-44-7, AL 106-49-0  
PRO AM 536742-05-9  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(43) OF 101 COMPOSED OF RX(2), RX(18)  
RX(43) C + AN ==> AO



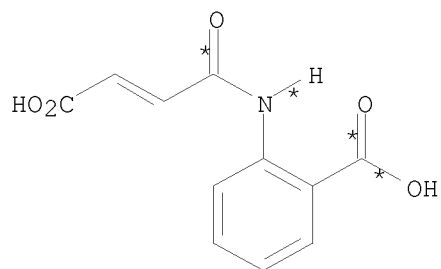
AO  
YIELD 68%

RX(2) RCT C 68040-76-6  
PRO D 107855-44-7  
CON 1 hour

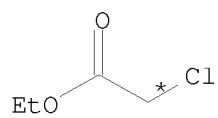
RX(18) RCT D 107855-44-7, AN 104-94-9  
PRO AO 536742-06-0  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(54) OF 101 COMPOSED OF RX(10), RX(6)  
RX(54) C + N ==> O

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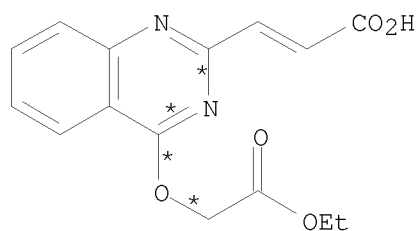


C



N

2  
STEPS  
→



O

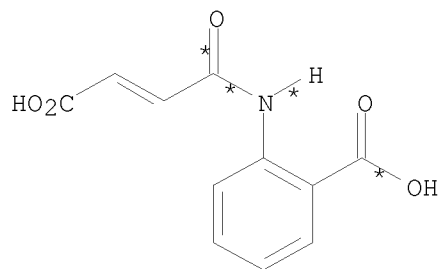
YIELD 62%

RX(10)     RCT   C 68040-76-6  
              RGT   Z 631-61-8 NH4OAc  
              PRO   M 5584-96-3  
              CON   1 hour, 170 deg C

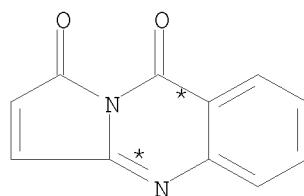
RX(6)       RCT   M 5584-96-3, N 105-39-5  
              RGT   P 584-08-7 K2CO3  
              PRO   O 536741-95-4  
              SOL   67-64-1 Me2CO  
              CON   24 hours

RX(55) OF 101 COMPOSED OF RX(10), RX(11)

RX(55)     C   +   AA   ==>   L



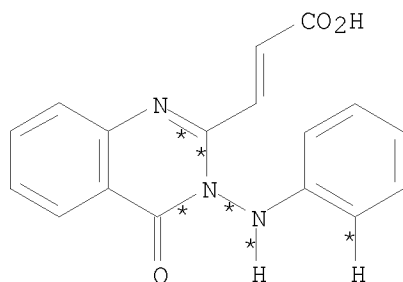
C



AA

2  
STEPS  
→

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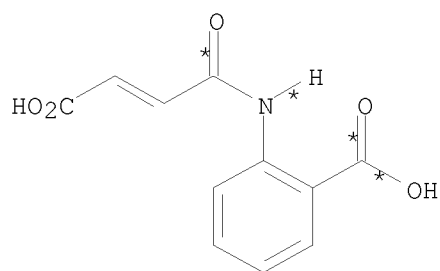


L  
YIELD 65%

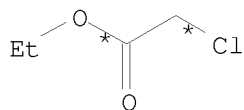
RX(10) RCT C 68040-76-6  
RGT Z 631-61-8 NH4OAc  
PRO M 5584-96-3  
CON 1 hour, 170 deg C

RX(11) RCT AA 536741-99-8, M 5584-96-3  
RGT AB 64-19-7 AcOH  
PRO L 5958-13-4  
SOL 64-19-7 AcOH  
CON SUBSTAGE(1) 80 deg C  
SUBSTAGE(2) 1 hour, 140 - 150 deg C  
NTE polyphosphoric acid

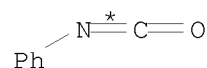
RX(74) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(9)  
RX(74) C + N + X ==> Y



C



N

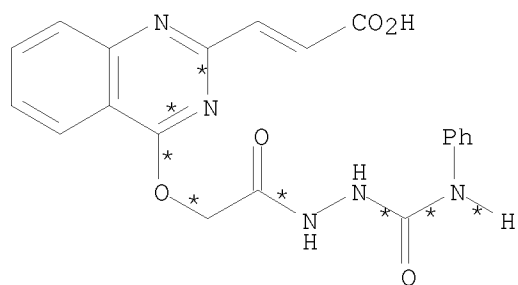


X

4

STEPS  
=>

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Y  
YIELD 63%

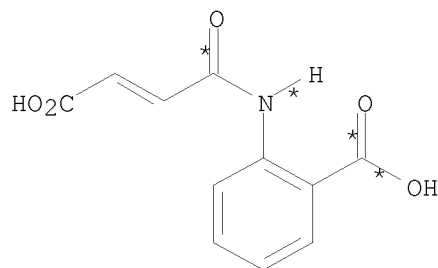
RX(10)      RCT    C 68040-76-6  
              RGT    Z 631-61-8 NH4OAc  
              PRO    M 5584-96-3  
              CON    1 hour, 170 deg C

RX(6)        RCT    M 5584-96-3, N 105-39-5  
              RGT    P 584-08-7 K2CO3  
              PRO    O 536741-95-4  
              SOL    67-64-1 Me2CO  
              CON    24 hours

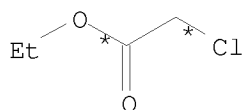
RX(8)        RCT    O 536741-95-4  
              RGT    W 302-01-2 N2H4  
              PRO    V 536741-97-6  
              SOL    64-17-5 EtOH  
              CON    3 hours, reflux

RX(9)        RCT    V 536741-97-6, X 103-71-9  
              PRO    Y 536741-98-7  
              SOL    64-17-5 EtOH  
              CON    4 hours, reflux

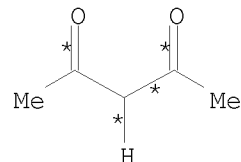
RX(75) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(12)  
RX(75)      C + N + AC ==> AD



C



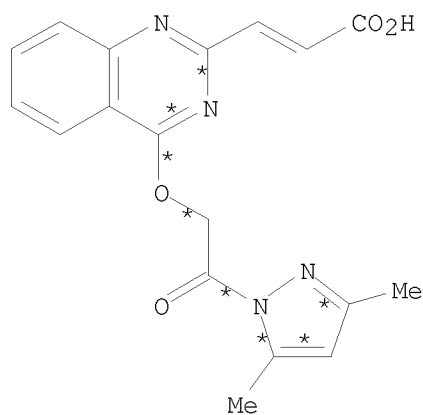
N



AC

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4  
STEPS  
→



AD  
YIELD 59%

RX(10)      RCT    C 68040-76-6  
              RGT    Z 631-61-8 NH<sub>4</sub>OAc  
              PRO    M 5584-96-3  
              CON    1 hour, 170 deg C

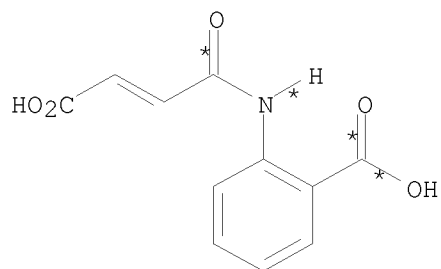
RX(6)        RCT    M 5584-96-3, N 105-39-5  
              RGT    P 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
              PRO    O 536741-95-4  
              SOL    67-64-1 Me<sub>2</sub>CO  
              CON    24 hours

RX(8)        RCT    O 536741-95-4  
              RGT    W 302-01-2 N<sub>2</sub>H<sub>4</sub>  
              PRO    V 536741-97-6  
              SOL    64-17-5 EtOH  
              CON    3 hours, reflux

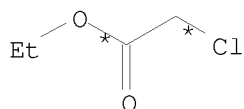
RX(12)       RCT    AC 123-54-6, V 536741-97-6  
              PRO    AD 536742-00-4  
              SOL    64-17-5 EtOH  
              CON    4 hours, reflux

RX(76) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(13)  
RX(76)      C + N + AE ==> AF

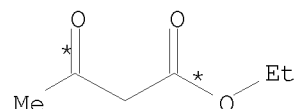
10/ 562,112



C

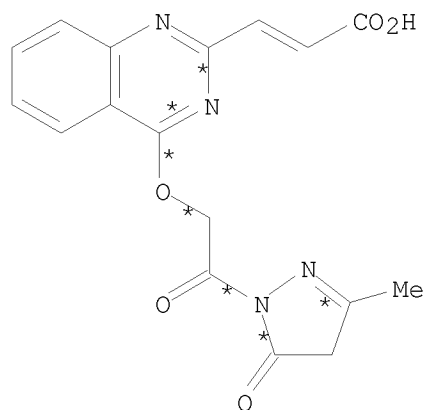


N



AE

4  
STEPS  
→

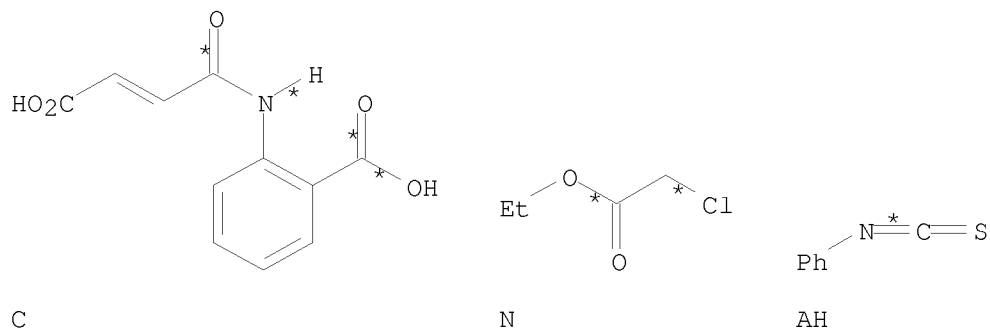


AF  
YIELD 60%

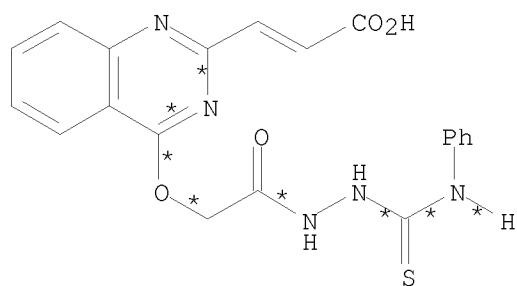
RX(10)	RCT	C 68040-76-6
	RGT	Z 631-61-8 NH4OAc
	PRO	M 5584-96-3
	CON	1 hour, 170 deg C
RX(6)	RCT	M 5584-96-3, N 105-39-5
	RGT	P 584-08-7 K2CO3
	PRO	O 536741-95-4
	SOL	67-64-1 Me2CO
RX(8)	CON	24 hours
	RCT	O 536741-95-4
	RGT	W 302-01-2 N2H4
	PRO	V 536741-97-6
RX(13)	SOL	64-17-5 EtOH
	CON	3 hours, reflux
	RCT	AE 141-97-9, V 536741-97-6
	PRO	AF 536742-01-5
	SOL	64-17-5 EtOH
	CON	4 hours, reflux

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RX(77) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(15)  
RX(77) C + N + AH ==> AI



4  
STEPS  
→



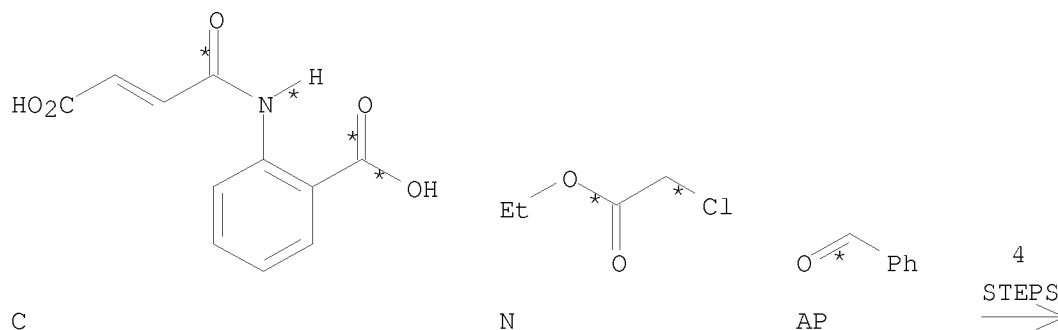
YIELD 60%

RX(10)	RCT	C 68040-76-6
	RGT	Z 631-61-8 NH4OAc
	PRO	M 5584-96-3
	CON	1 hour, 170 deg C
RX(6)	RCT	M 5584-96-3, N 105-39-5
	RGT	P 584-08-7 K2CO3
	PRO	O 536741-95-4
	SOL	67-64-1 Me2CO
	CON	24 hours
RX(8)	RCT	O 536741-95-4
	RGT	W 302-01-2 N2H4
	PRO	V 536741-97-6
	SOL	64-17-5 EtOH
	CON	3 hours, reflux
RX(15)	RCT	V 536741-97-6, AH 103-72-0
	PRO	AI 536742-03-7

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SOL 64-17-5 EtOH  
CON 4 hours, reflux

RX(78) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(19)  
RX(78) C + N + AP ==> AQ



AQ  
YIELD 60%

RX(10) RCT C 68040-76-6  
RGT Z 631-61-8 NH4OAc  
PRO M 5584-96-3  
CON 1 hour, 170 deg C

RX(6) RCT M 5584-96-3, N 105-39-5  
RGT P 584-08-7 K2CO3  
PRO O 536741-95-4  
SOL 67-64-1 Me2CO  
CON 24 hours

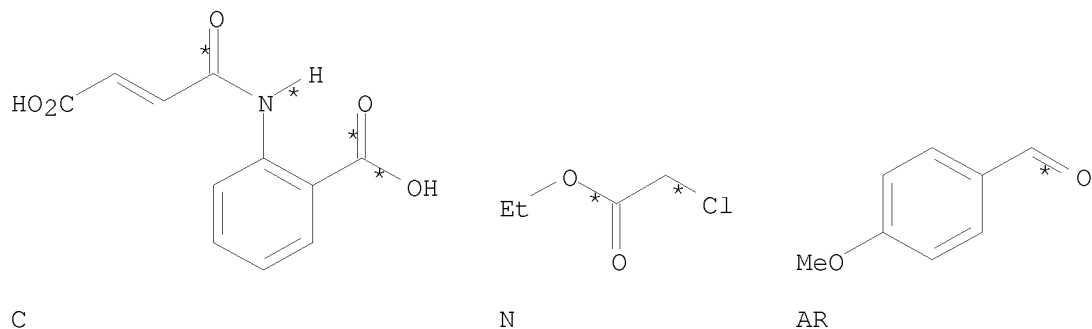
RX(8) RCT O 536741-95-4  
RGT W 302-01-2 N2H4  
PRO V 536741-97-6  
SOL 64-17-5 EtOH  
CON 3 hours, reflux

RX(19) RCT V 536741-97-6, AP 100-52-7  
PRO AQ 536742-07-1  
SOL 64-17-5 EtOH  
CON 3 hours, reflux

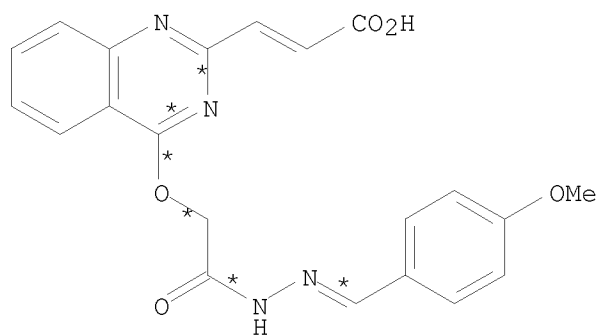


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RX(79) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(20)  
RX(79) C + N + AR ==> AS



4  
STEPS  
→



AS  
YIELD 65%

RX(10) RCT C 68040-76-6  
RGT Z 631-61-8 NH4OAc  
PRO M 5584-96-3  
CON 1 hour, 170 deg C

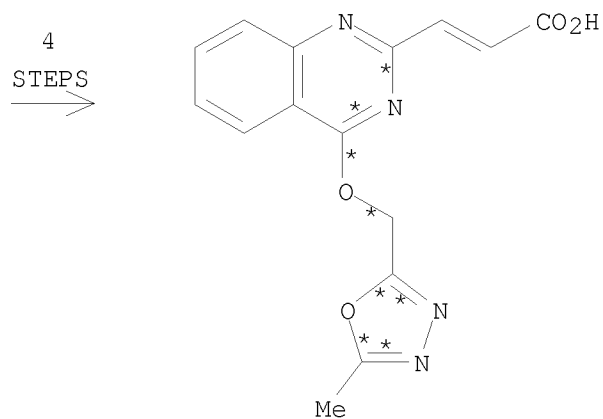
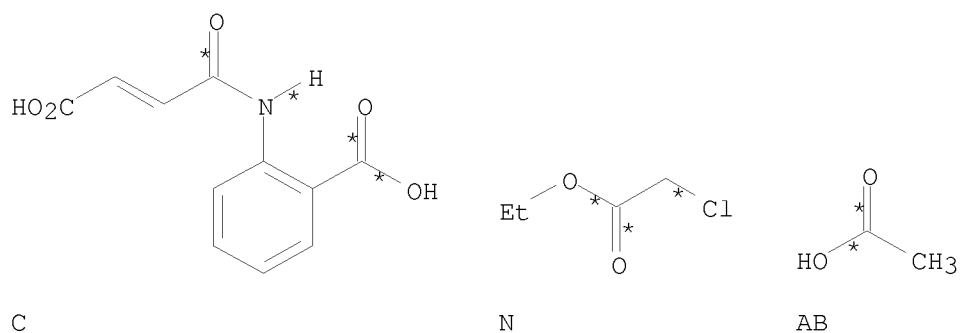
RX(6) RCT M 5584-96-3, N 105-39-5  
RGT P 584-08-7 K2CO3  
PRO O 536741-95-4  
SOL 67-64-1 Me2CO  
CON 24 hours

RX(8) RCT O 536741-95-4  
RGT W 302-01-2 N2H4  
PRO V 536741-97-6  
SOL 64-17-5 EtOH  
CON 3 hours, reflux

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RX(20) RCT V 536741-97-6, AR 123-11-5  
PRO AS 536742-08-2  
SOL 64-17-5 EtOH  
CON 3 hours, reflux

RX(80) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(23)  
RX(80) C + N + AB ==> AW



AW  
YIELD 70%

RX(10) RCT C 68040-76-6  
RGT Z 631-61-8 NH4OAc  
PRO M 5584-96-3  
CON 1 hour, 170 deg C

RX(6) RCT M 5584-96-3, N 105-39-5  
RGT P 584-08-7 K2CO3  
PRO O 536741-95-4  
SOL 67-64-1 Me2CO  
CON 24 hours

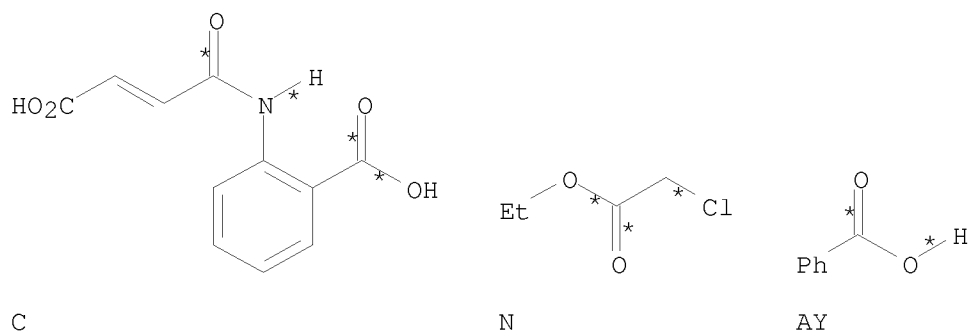
RX(8) RCT O 536741-95-4  
RGT W 302-01-2 N2H4  
PRO V 536741-97-6

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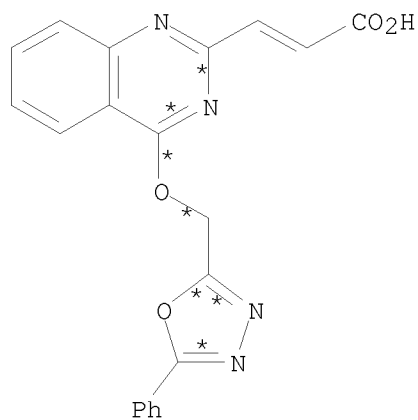
SOL 64-17-5 EtOH  
CON 3 hours, reflux

RX(23) RCT AB 64-19-7, V 536741-97-6  
RGT AX 10025-87-3 POC13  
PRO AW 536742-11-7  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

RX(81) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(24)  
RX(81) C + N + AY ==> AZ



4  
STEPS  
→



AZ  
YIELD 71%

RX(10) RCT C 68040-76-6  
RGT Z 631-61-8 NH4OAc  
PRO M 5584-96-3  
CON 1 hour, 170 deg C

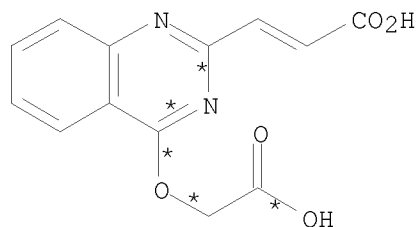
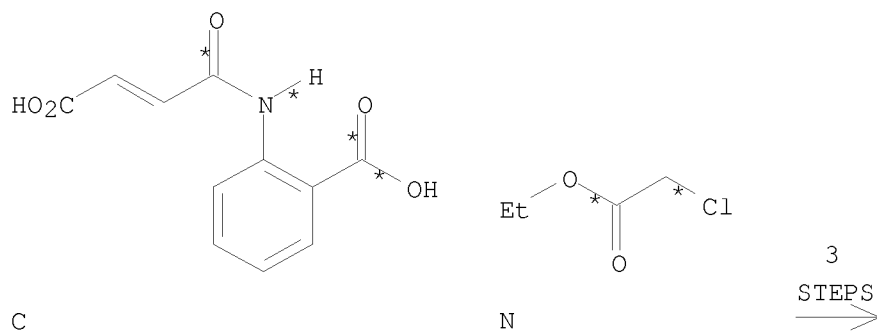
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RX(6)      RCT    M 5584-96-3, N 105-39-5  
             RGT    P 584-08-7 K2CO3  
             PRO    O 536741-95-4  
             SOL    67-64-1 Me2CO  
             CON    24 hours

RX(8)      RCT    O 536741-95-4  
             RGT    W 302-01-2 N2H4  
             PRO    V 536741-97-6  
             SOL    64-17-5 EtOH  
             CON    3 hours, reflux

RX(24)     RCT    AY 65-85-0, V 536741-97-6  
             RGT    AX 10025-87-3 POC13  
             PRO    AZ 536742-12-8  
             SOL    64-17-5 EtOH  
             CON    5 hours, reflux

RX(86) OF 101 COMPOSED OF RX(10), RX(6), RX(7)  
RX(86)      C    +    N    ==>    R



R  
YIELD 70%

RX(10)     RCT    C 68040-76-6  
             RGT    Z 631-61-8 NH4OAc  
             PRO    M 5584-96-3  
             CON    1 hour, 170 deg C

RX(6)      RCT    M 5584-96-3, N 105-39-5  
             RGT    P 584-08-7 K2CO3

10/ 562,112

PRO O 536741-95-4  
SOL 67-64-1 Me2CO  
CON 24 hours

RX(7) RCT O 536741-95-4

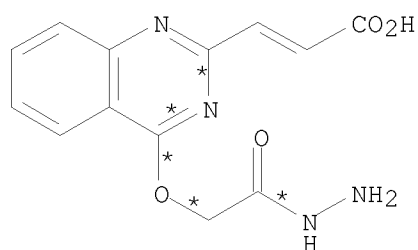
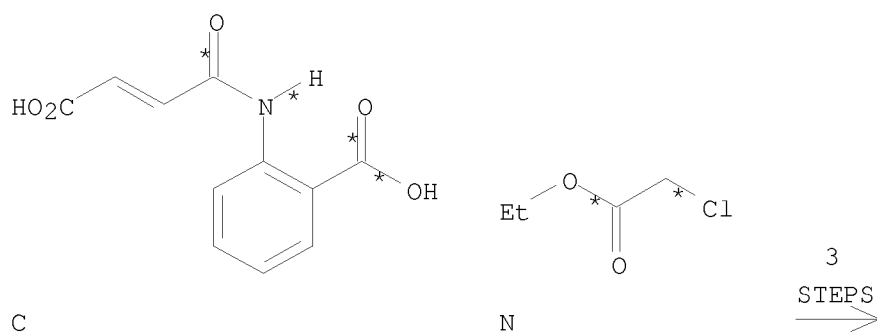
STAGE(1)  
RGT S 1310-73-2 NaOH  
SOL 7732-18-5 Water  
CON 3 hours, reflux

STAGE(2)  
RGT T 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO R 536741-96-5

RX(87) OF 101 COMPOSED OF RX(10), RX(6), RX(8)

RX(87) C + N ==> V



V  
YIELD 67%

RX(10) RCT C 68040-76-6  
RGT Z 631-61-8 NH4OAc  
PRO M 5584-96-3  
CON 1 hour, 170 deg C

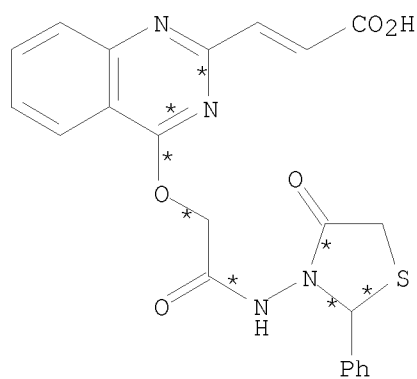
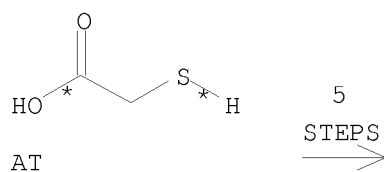
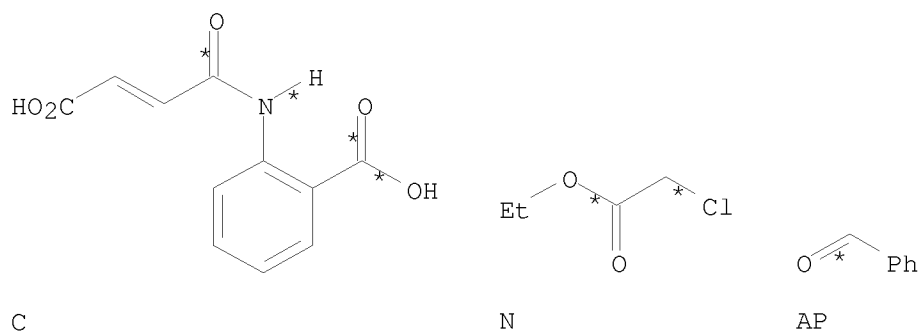
RX(6) RCT M 5584-96-3, N 105-39-5  
RGT P 584-08-7 K2CO3  
PRO O 536741-95-4

10/ 562,112

SOL 67-64-1 Me<sub>2</sub>CO  
CON 24 hours

RX(8) RCT O 536741-95-4  
RGT W 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO V 536741-97-6  
SOL 64-17-5 EtOH  
CON 3 hours, reflux

RX(98) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(19), RX(21)  
RX(98) C + N + AP + AT ==> AU



AU  
YIELD 61%

RX(10) RCT C 68040-76-6  
RGT Z 631-61-8 NH<sub>4</sub>OAc  
PRO M 5584-96-3  
CON 1 hour, 170 deg C

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RX(6) RCT M 5584-96-3, N 105-39-5  
RGT P 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO O 536741-95-4  
SOL 67-64-1 Me<sub>2</sub>CO  
CON 24 hours

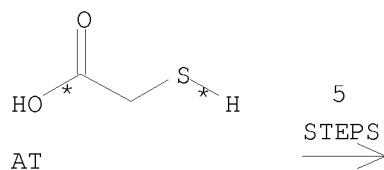
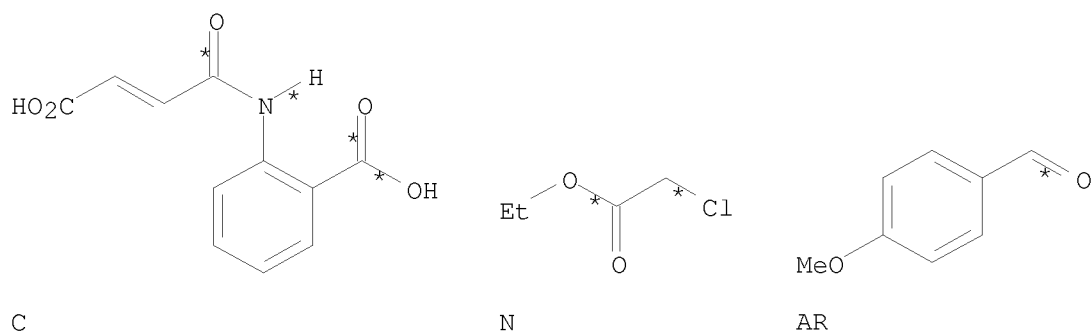
RX(8) RCT O 536741-95-4  
RGT W 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO V 536741-97-6  
SOL 64-17-5 EtOH  
CON 3 hours, reflux

RX(19) RCT V 536741-97-6, AP 100-52-7  
PRO AQ 536742-07-1  
SOL 64-17-5 EtOH  
CON 3 hours, reflux

RX(21) RCT AQ 536742-07-1, AT 68-11-1  
PRO AU 536742-09-3  
SOL 64-17-5 EtOH  
CON 3 hours, reflux

RX(99) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(20), RX(22)

RX(99) C + N + AR + AT ==> AV



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(10) RCT C 68040-76-6  
RGT Z 631-61-8 NH<sub>4</sub>OAc  
PRO M 5584-96-3  
CON 1 hour, 170 deg C

RX(6) RCT M 5584-96-3, N 105-39-5

RGT P 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO O 536741-95-4  
 SOL 67-64-1 Me<sub>2</sub>CO  
 CON 24 hours

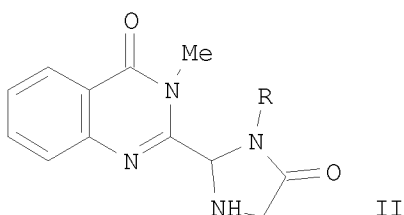
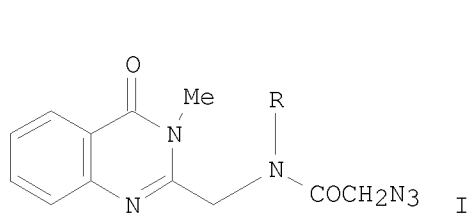
RX(8) RCT O 536741-95-4  
 RGT W 302-01-2 N<sub>2</sub>H<sub>4</sub>  
 PRO V 536741-97-6  
 SOL 64-17-5 EtOH  
 CON 3 hours, reflux

RX(20) RCT V 536741-97-6, AR 123-11-5  
 PRO AS 536742-08-2  
 SOL 64-17-5 EtOH  
 CON 3 hours, reflux

RX(22) RCT AS 536742-08-2, AT 68-11-1  
 PRO AV 536742-10-6  
 SOL 64-17-5 EtOH  
 CON 3 hours, reflux

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 88 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 139:6837 CASREACT  
 TITLE: Synthesis of 2-quinazolinonyl imidazolidinones  
 AUTHOR(S): Reddy, P. S. N.; Reddy, P. Pratap; Vasantha, T.  
 CORPORATE SOURCE: Dep. of Chem., Osmania Univ., Hyderabad, 500 007, India  
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2003), 42B(2), 393-396  
 CODEN: IJSBDB; ISSN: 0376-4699  
 PUBLISHER: National Institute of Science Communication  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

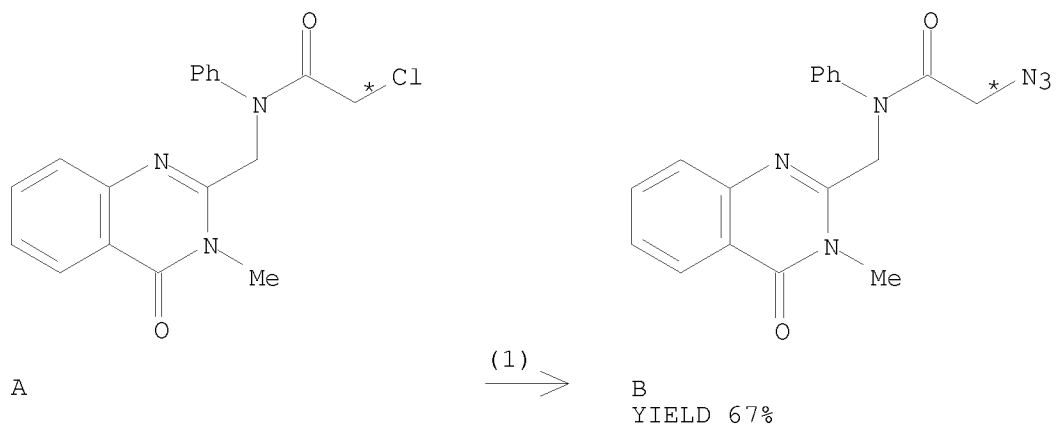


AB 2-Chloromethyl-3-methylquinazolin-4(3H)-one is converted to azides I (R = Ph, substituted Ph) which easily undergoes cyclization to give 2-quinazolinonyl imidazolidinones II. I (R = p-MeC<sub>6</sub>H<sub>4</sub>), however, yield 2,3-dimethylquinazolin-4(3H)-one and/or 2-(p-tolylaminomethyl)-3-methylquinazolin-4(3H)-one under thermal, microwave and in acidic medium.



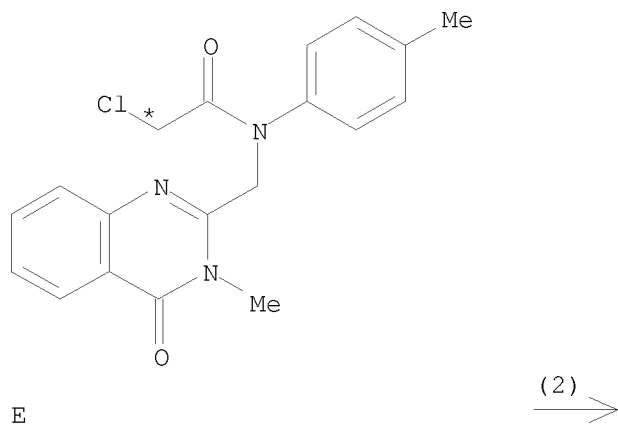
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RX(1) OF 15      A    ==>   B...

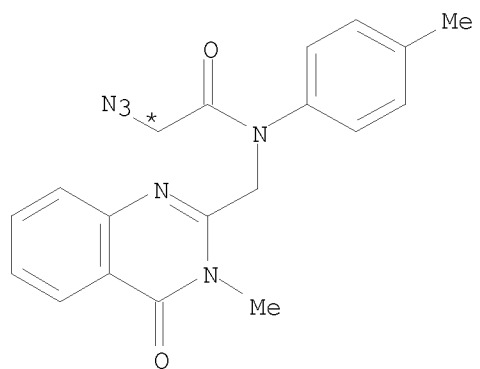


RX(1)      RCT    A 228871-37-2  
             RGT    C 26628-22-8 NaN<sub>3</sub>  
             PRO    B 536697-61-7  
             SOL    68-12-2 DMF  
             CON    1 hour, room temperature

RX(2) OF 15      E    ==>   F...



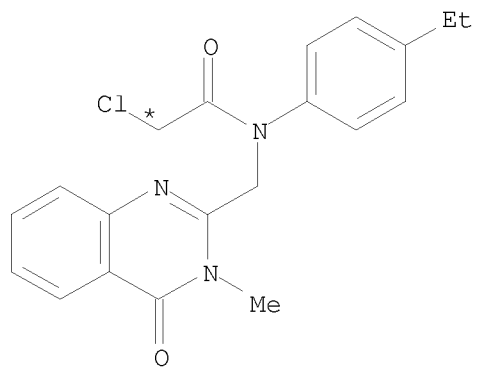
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F  
YIELD 80%

RX(2)      RCT   E 228871-38-3  
             RGT   C 26628-22-8 NaN<sub>3</sub>  
             PRO   F 536697-62-8  
             SOL   68-12-2 DMF  
             CON   1 hour, room temperature

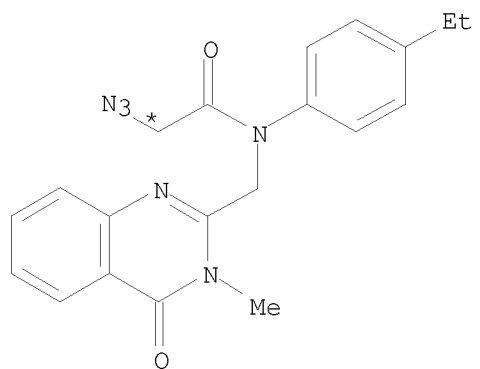
RX(3) OF 15      G   ==>   H...



G

(3) →

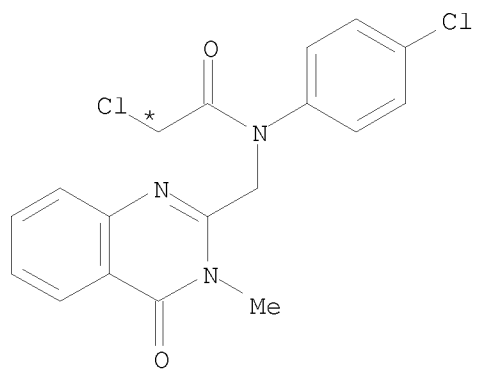
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H  
YIELD 79%

RX(3)      RCT    G 228871-40-7  
             RGT    C 26628-22-8 NaN3  
             PRO    H 536697-63-9  
             SOL    68-12-2 DMF  
             CON    1 hour, room temperature

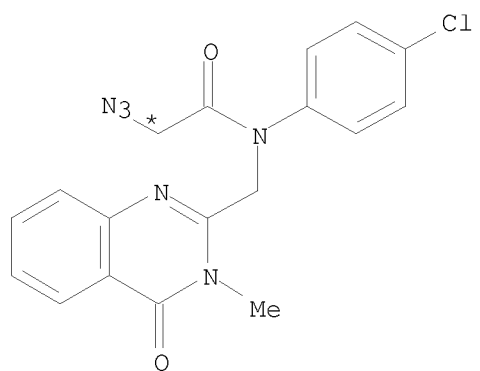
RX(4) OF 15      I    ==>    J...



I

(4)  $\longrightarrow$

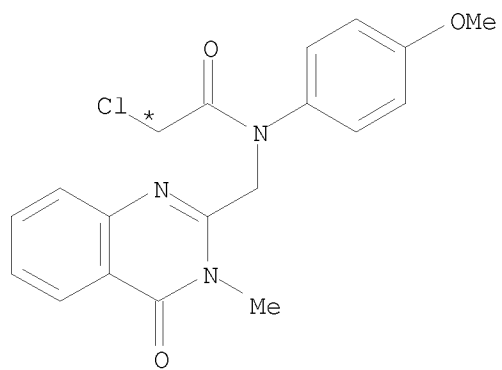
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J  
YIELD 90%

RX(4)      RCT    I 228871-41-8  
             RGT    C 26628-22-8 NaN3  
             PRO    J 536697-64-0  
             SOL    68-12-2 DMF  
             CON    1 hour, room temperature

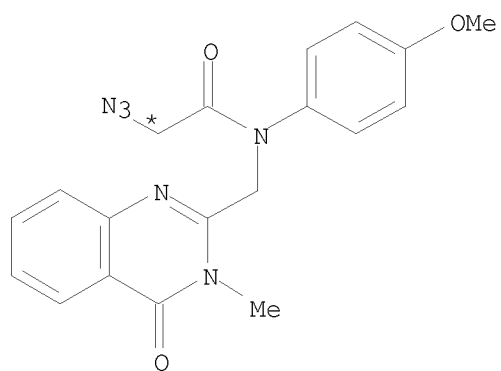
RX(5) OF 15      K ==> L



K

(5) →

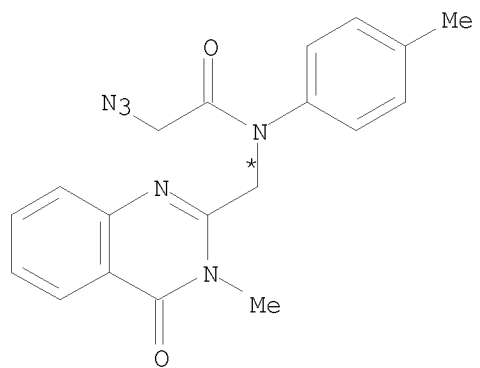
10/ 562,112



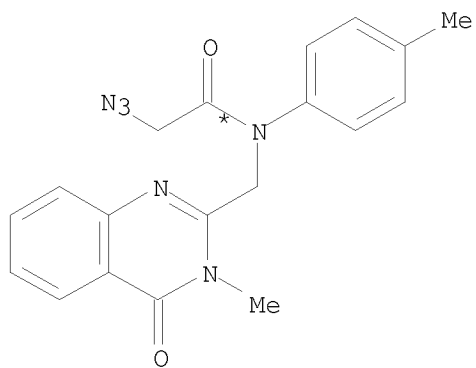
L  
YIELD 72%

RX(5)      RCT   K 228871-39-4  
             RGT   C 26628-22-8 NaN<sub>3</sub>  
             PRO   L 536697-65-1  
             SOL   68-12-2 DMF  
             CON   1 hour, room temperature

RX(10) OF 15      ...2 F ==> S + T



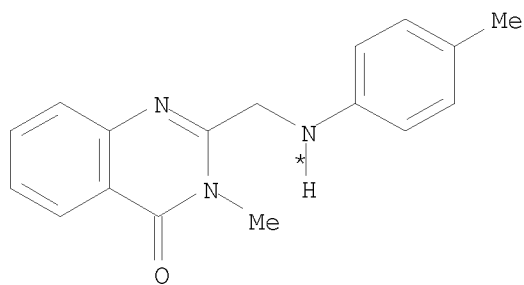
F



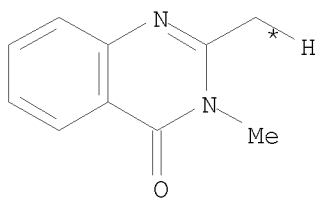
F

(10)  
→

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S  
YIELD 20%

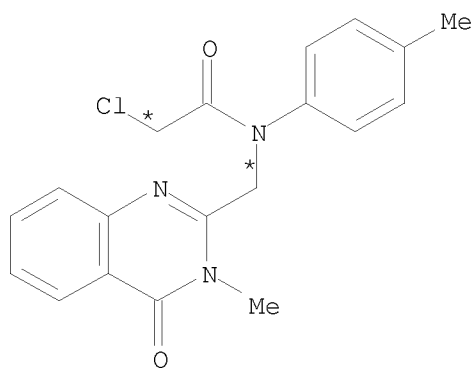


T  
YIELD 50%

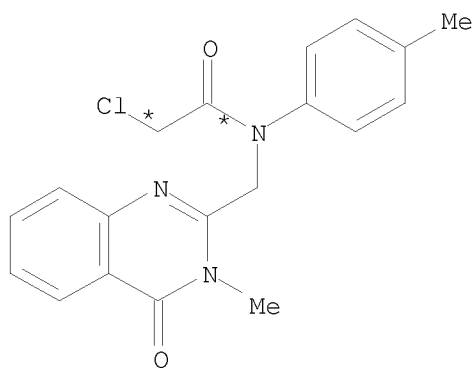
RX(10)      RCT    F 536697-62-8  
              RGT    U 1493-13-6 F3CSO2H  
              PRO    S 228871-31-6, T 1769-25-1  
              SOL    75-09-2 CH2Cl2  
              CON    40 hours, room temperature

RX(13) OF 15 COMPOSED OF RX(2), RX(10)

RX(13)      2 E    ==>    S   +   T

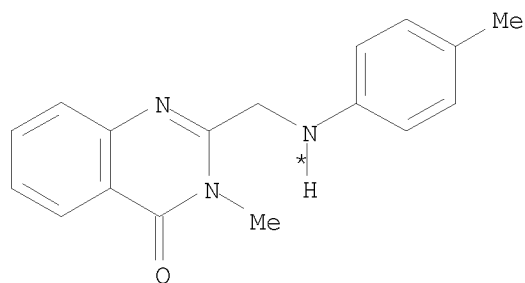


E

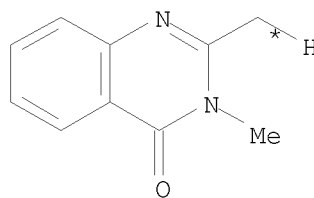


E

2  
STEPS  
=>



S  
YIELD 20%



T  
YIELD 50%

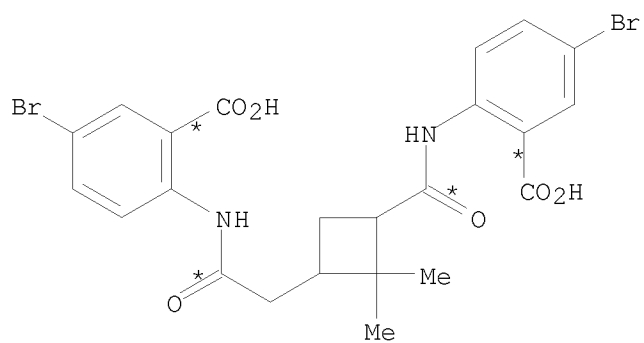
RX(2) RCT E 228871-38-3  
RGT C 26628-22-8 NaN3  
PRO F 536697-62-8  
SOL 68-12-2 DMF  
CON 1 hour, room temperature

RX(10) RCT F 536697-62-8  
RGT U 1493-13-6 F3CSO2H  
PRO S 228871-31-6, T 1769-25-1  
SOL 75-09-2 CH2Cl2  
CON 40 hours, room temperature

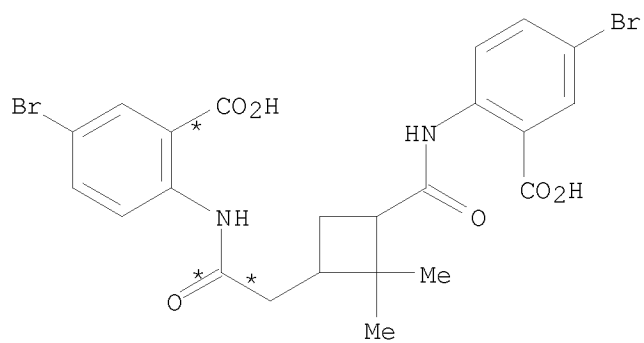
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 89 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 138:338095 CASREACT  
TITLE: Di-6R, 7R1-4(3H)-oxo-2-quinazolinyl-substituted cyclobutanes from pinic and sym-homopinic acids  
AUTHOR(S): Avotin'sh, F.; Petrova, M.; Strakovs, A.  
CORPORATE SOURCE: Riga Technical University, Riga, LV-1658, Latvia  
SOURCE: Chemistry of Heterocyclic Compounds (New York, NY, United States)(Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2002), 38(7), 817-821  
CODEN: CHCCAL; ISSN: 0009-3122  
PUBLISHER: Kluwer Academic/Consultants Bureau  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Diamides were obtained by reaction of cis-3-carboxy-2,2-dimethylcyclobutylacetic acid (pinic acid) and of cis/trans-3-(carboxymethyl)-2,2-dimethylcyclobutylacetic acid (homopinic acid) dichlorides with two equivalent of 5-bromo-, 4-chloro-, and 4,5-dimethoxyanthranilic acids. Treatment of the diamides with formamide leads to 2,2-dimethyl-3-[4(3H)-oxo-2-quinazolinyl]methyl-1-[4(3H)-oxo-2-quinazolinyl]cyclobutanes and 2,2-dimethyl-1,3-di[4(3H)-oxo-2-quinazolinylmethyl]cyclobutanes.

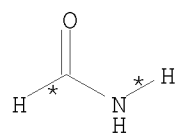
RX(7) OF 18 ...2 C + 3 N ==> O + P



C

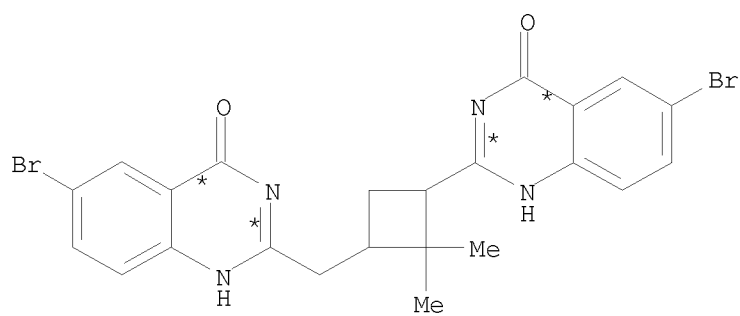


C



3 N

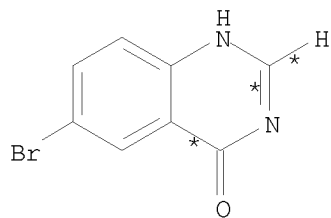
(7) →



O  
YIELD 50%



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P  
YIELD 22%

RX(7) RCT C 517915-11-6, N 75-12-7

STAGE(1)

SOL 75-12-7 Formamide

CON SUBSTAGE(1) 2 hours, 180 - 185 deg C

SUBSTAGE(2) 185 deg C -> room temperature

STAGE(2)

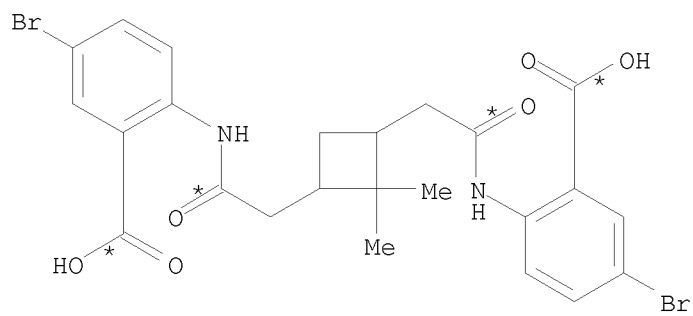
RGT Q 144-55-8 NaHCO3

SOL 7732-18-5 Water

CON room temperature

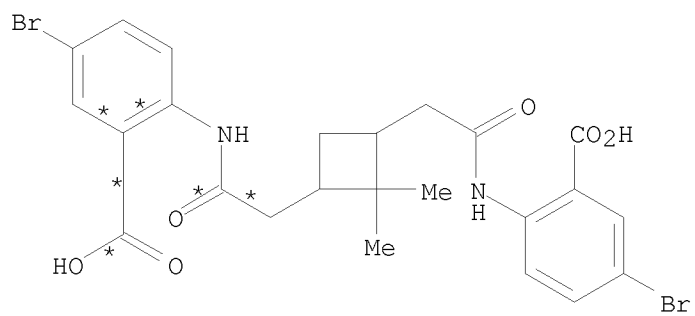
PRO O 517915-17-2, P 32084-59-6

RX(10) OF 18 ...3 K + 3 N ==> W + P

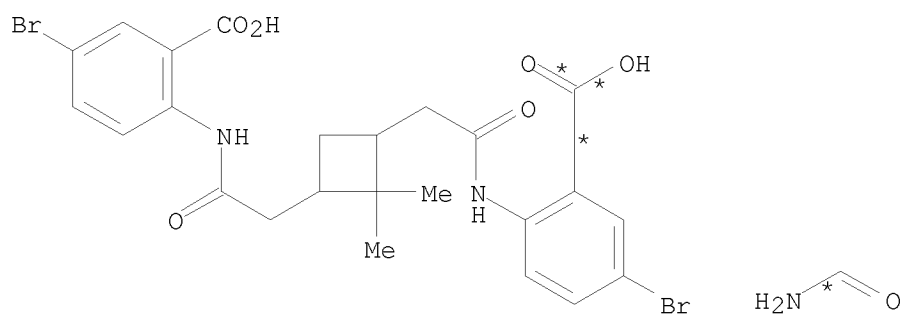


K

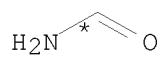
10/ 562,112



K

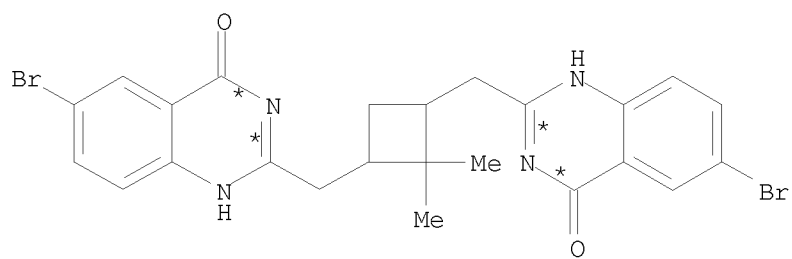


K



3 N

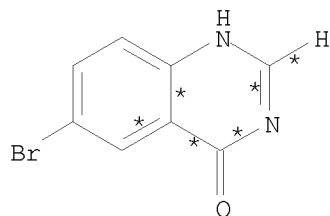
(10)



W

YIELD 48%

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P  
YIELD 19%

RX(10) RCT K 517915-14-9, N 75-12-7

STAGE(1)

SOL 75-12-7 Formamide

CON SUBSTAGE(1) 2 hours, 186 deg C

SUBSTAGE(2) 186 deg C -> room temperature

STAGE(2)

RGT Q 144-55-8 NaHCO3

SOL 7732-18-5 Water

CON room temperature

PRO W 517915-20-7, P 32084-59-6

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 90 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 138:271640 CASREACT

TITLE: Synthesis of some new quinazoline-4-(3H)-ones and  
styryl hemicyanines as possible antimicrobial agents

AUTHOR(S): Afsah, S. A.; Ahmad, Jawaid; Purbey, R.; Kumar, A.

CORPORATE SOURCE: Post-graduate Department of Chemistry, R.K. College,  
Madhubani, 847 211, India

SOURCE: Asian Journal of Chemistry (2003), 15(1), 552-554

CODEN: AJCHEW; ISSN: 0970-7077

PUBLISHER: Asian Journal of Chemistry

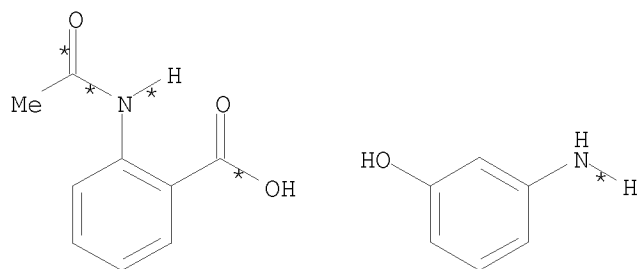
DOCUMENT TYPE: Journal

LANGUAGE: English

AB In the present note we report the synthesis of some new quinazoline-4  
(3H)-ones and styryl hemicyanines as possible antimicrobial agents. The  
preparation and properties of the title styryl hemicyanines were not reported.

RX(2) OF 15 ...C + D ==> E

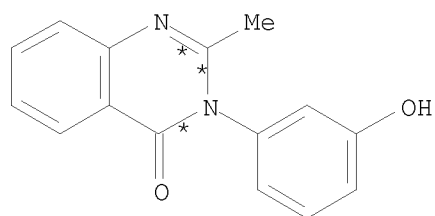
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C

D

(2)  $\longrightarrow$



E

YIELD 68%

RX(2)

RCT C 89-52-1

STAGE(1)

SOL 108-24-7 Ac2O

CON 4 - 6 hours, reflux

STAGE(2)

RCT D 591-27-5

SOL 64-19-7 AcOH

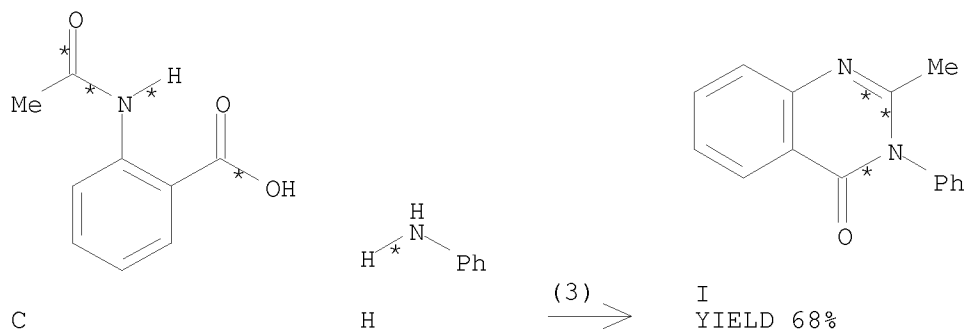
CON 4 - 6 hours, reflux

PRO E 40671-68-9

RX(3) OF 15

...C + H ==> I

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RX(3) RCT C 89-52-1

STAGE(1)

SOL 108-24-7 Ac2O

CON 4 - 6 hours, reflux

STAGE(2)

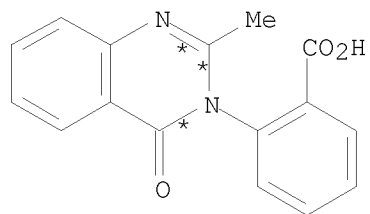
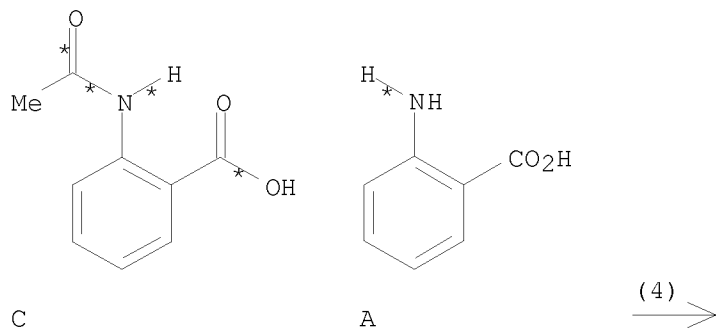
RCT H 62-53-3

SOL 64-19-7 AcOH

CON 4 - 6 hours, reflux

PRO I 2385-23-1

RX(4) OF 15 ...C + A ==> J



J  
YIELD 68%

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RX(4) RCT C 89-52-1

STAGE(1)

SOL 108-24-7 Ac2O

CON 4 - 6 hours, reflux

STAGE(2)

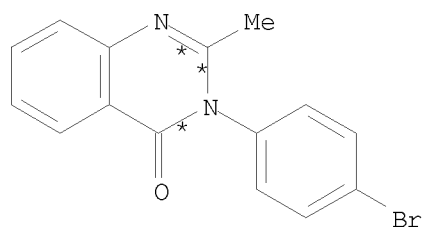
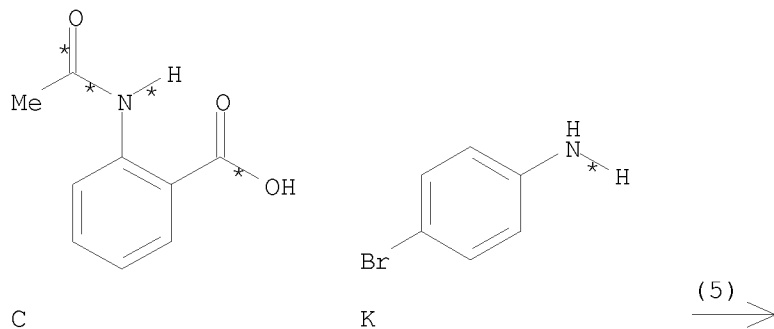
RCT A 118-92-3

SOL 64-19-7 AcOH

CON 4 - 6 hours, reflux

PRO J 4005-06-5

RX(5) OF 15 ...C + K ==> L



L  
YIELD 68%

RX(5) RCT C 89-52-1

STAGE(1)

SOL 108-24-7 Ac2O

CON 4 - 6 hours, reflux

STAGE(2)

RCT K 106-40-1

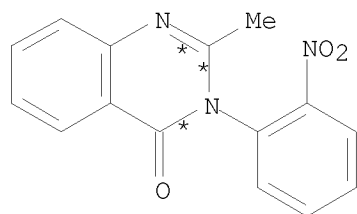
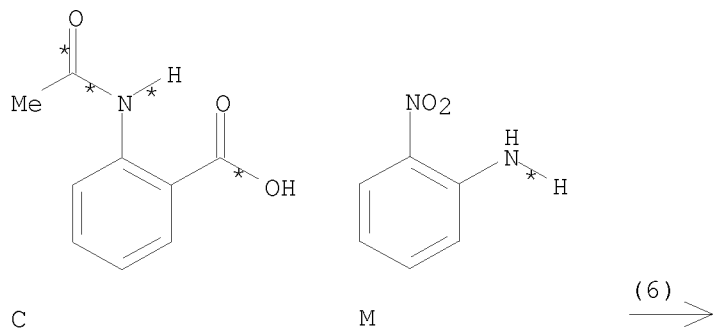
SOL 64-19-7 AcOH

CON 4 - 6 hours, reflux

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PRO L 1788-95-0

RX(6) OF 15 ...C + M ==> N



N  
YIELD 68%

RX(6) RCT C 89-52-1

STAGE(1)

SOL 108-24-7 Ac2O

CON 4 - 6 hours, reflux

STAGE(2)

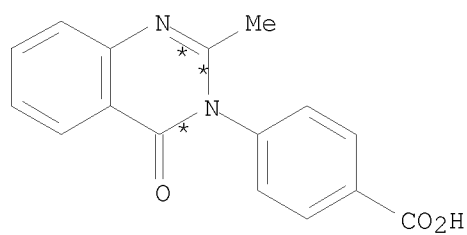
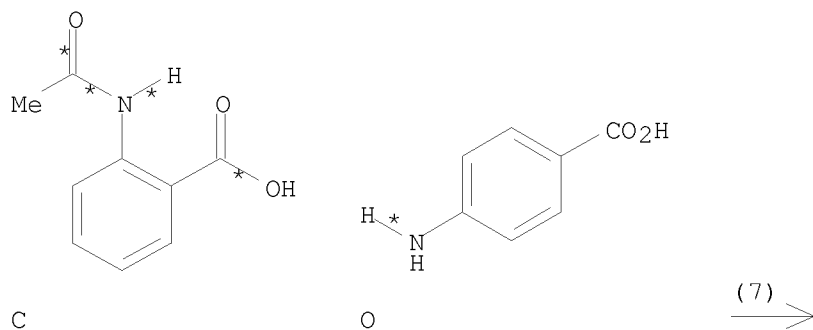
RCT M 88-74-4

SOL 64-19-7 AcOH

CON 4 - 6 hours, reflux

PRO N 1788-94-9

RX(7) OF 15 ...C + O ==> P



P  
YIELD 68%

RX(7) RCT C 89-52-1

STAGE(1)

SOL 108-24-7 Ac2O

CON 4 - 6 hours, reflux

STAGE(2)

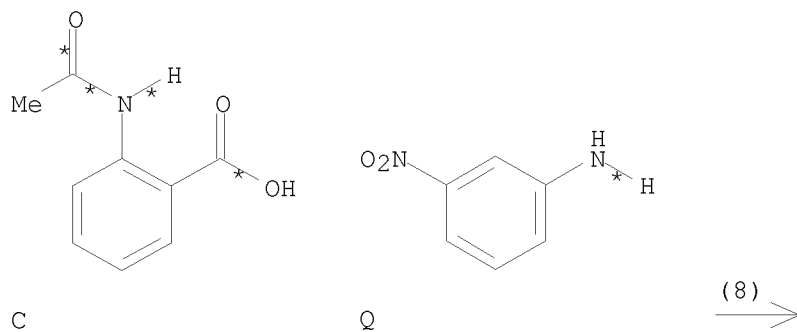
RCT O 150-13-0

SOL 64-19-7 AcOH

CON 4 - 6 hours, reflux

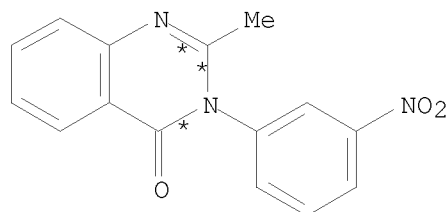
PRO P 4005-05-4

RX(8) OF 15 ...C + Q ==> R





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R  
YIELD 68%

RX(8) RCT C 89-52-1

STAGE(1)

SOL 108-24-7 Ac2O  
CON 4 - 6 hours, reflux

STAGE(2)

RCT Q 99-09-2  
SOL 64-19-7 AcOH  
CON 4 - 6 hours, reflux

PRO R 4309-26-6

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 91 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 138:239381 CASREACT

TITLE: Synthesis and application of some bisazo disperse dyes  
based on 4-hydroxyquinolinoquinazoline system on  
polyester fabric

AUTHOR(S): Patel, N. C.; Mehta, A. G.

CORPORATE SOURCE: Department of Chemistry, P.T. Sarvajani College of  
Science, Surat, 395 001, India

SOURCE: Journal of Indian Council of Chemists (2001), 18(2),  
83-86

CODEN: JICCE7; ISSN: 0971-5037

PUBLISHER: Indian Council of Chemists

DOCUMENT TYPE: Journal

LANGUAGE: English

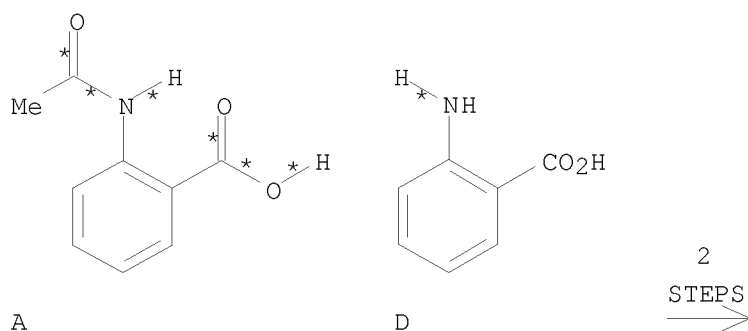
AB Ten 3-(4'-R-azo-1'-phenylazo)-4-hydroxyquinolino-[1,2-b]-4-oxoquinazolines  
were prepared by coupling diazotized  
3-(4'-amino-1'-phenylazo)-4-hydroxyquinolino-[1,2-b]-4-oxoquinazoline with  
various coupling components. 4-Hydroxyquinolino-[1,2-b]-4-oxoquinazoline  
(I) was prepared by the condensation of 2-methyl-1,3-benzoxazin-8-one with  
anthranilic acid, giving initially  
2-methyl-3-(1-carboxyphenyl)-4-oxoquinazoline followed by the ring  
closure. I was coupled with diazotized p-aminoacetanilide followed by  
hydrolysis to give 3-[4'-amino-1'-phenylazo]-4-hydroxyquinolino[1,2-b]-4-  
oxoquinazoline. The bisazo disperse dyes were characterized by elemental  
and spectral analyses and their dyeing performance on polyester fabric was

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assessed. These compds. when applied on polyester fabric, gave shades with poor to good light fastness, very good to excellent wash fastness and poor to excellent exhaustion.

RX(16) OF 75 COMPOSED OF RX(1), RX(2)

RX(16) A + D ==> E



E  
YIELD 85%

RX(1) RCT A 89-52-1  
RGT C 108-24-7 Ac2O  
PRO B 525-76-8  
CON 30 minutes, reflux

RX(2) RCT B 525-76-8, D 118-92-3  
PRO E 4005-06-5  
SOL 64-19-7 AcOH  
CON 3 hours, reflux

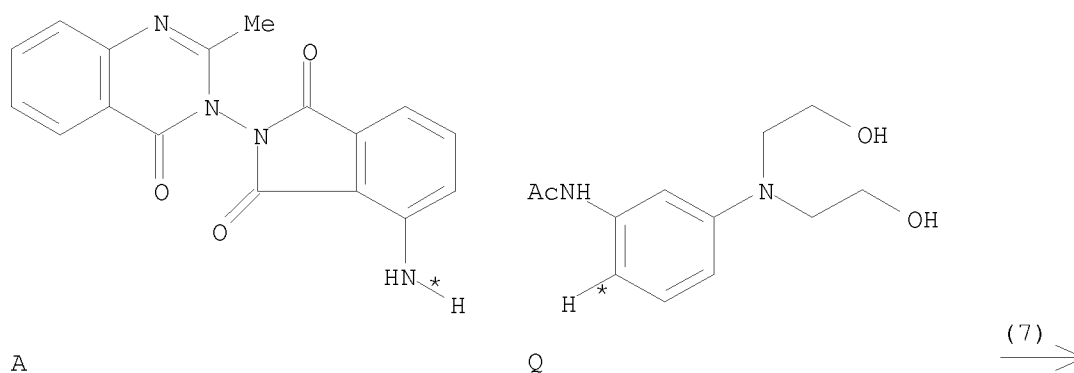
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 92 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 138:206465 CASREACT  
TITLE: Disperse dyes based on  
2-methyl-3-[[3'-(aminophthalimido)]-4(3H)-quinazolinone  
AUTHOR(S): Patel, Vijay H.; Patel, Manish P.; Patel, Ranjan G.

CORPORATE SOURCE: Department of Chemistry, Sardar Patel University,  
Vallabh Vidyanagar, 388 120, India  
SOURCE: Journal of the Serbian Chemical Society (2002),  
67(11), 719-726  
CODEN: JSCSEN; ISSN: 0352-5139  
PUBLISHER: Serbian Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Azo heterocyclic disperse dyes were prepared by diazotization of 3-(3-aminophthalimido)-2-methyl-4(3H)-quinazolinone and coupling with 14 different mono- and di-N-substituted aniline derivs. The yellow to brown dyes were characterized by their percentage yield, m.p., UV-visible spectra, elemental anal., IR spectra, and dyeing performance on nylon 66 and polyester fibers. The percentage dye bath exhaustion was reasonably good and acceptable. The dyed fibers showed fair to fairly good to good fastness to light and very good to excellent fastness to washing, rubbing, perspiration, and sublimation.

RX(7) OF 29 ...A + Q ==> R



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(7) RCT A 500226-05-1

STAGE(1)

RGT D 7632-00-0 NaNO<sub>2</sub>, E 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 0 - 5 deg C

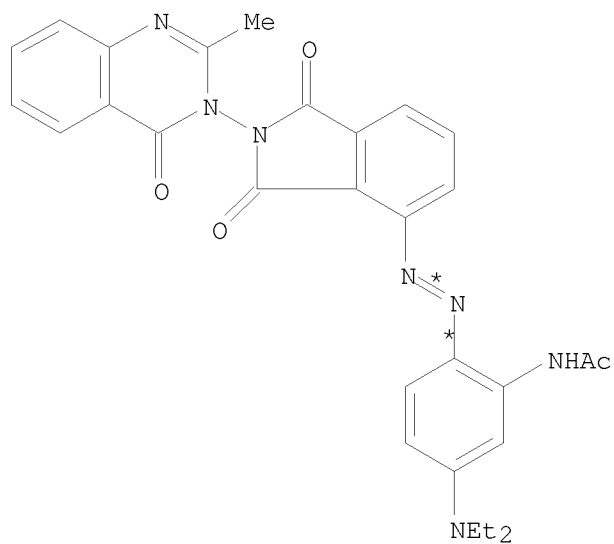
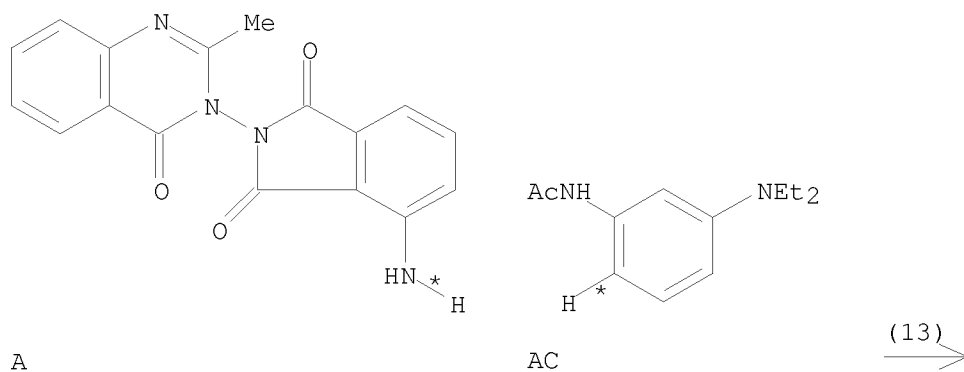
STAGE(2)

RCT Q 92-02-4  
RGT E 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 45 minutes, 0 - 5 deg C  
SUBSTAGE(2) 24 hours, 0 - 5 deg C, pH 5 - 6

PRO R 500225-96-7

RX(13) OF 29 ...A + AC ==> AD

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AD  
YIELD 75%

RX(13) RCT A 500226-05-1

STAGE(1)

RGT D 7632-00-0 NaNO<sub>2</sub>, E 7647-01-0 HCl

SOL 7732-18-5 Water

CON 0 - 5 deg C

STAGE(2)

RCT AC 6375-46-8

RGT E 7647-01-0 HCl

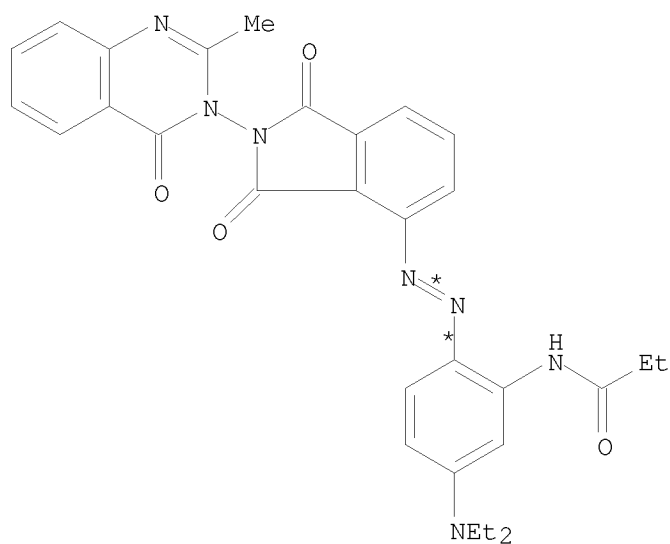
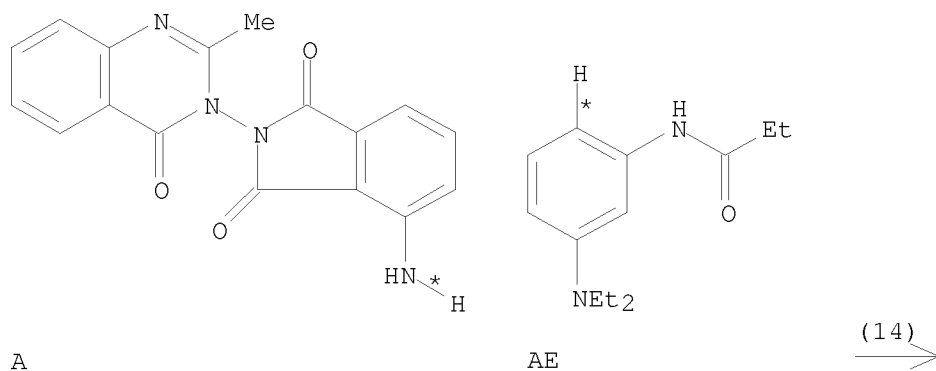
SOL 7732-18-5 Water

CON SUBSTAGE(1) 45 minutes, 0 - 5 deg C

SUBSTAGE(2) 24 hours, 0 - 5 deg C, pH 5 - 6

PRO AD 500226-02-8

RX(14) OF 29 ...A + AE ==> AF



AF  
YIELD 70%

RX(14) RCT A 500226-05-1

STAGE(1)

RGT D 7632-00-0 NaNO<sub>2</sub>, E 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 0 - 5 deg C

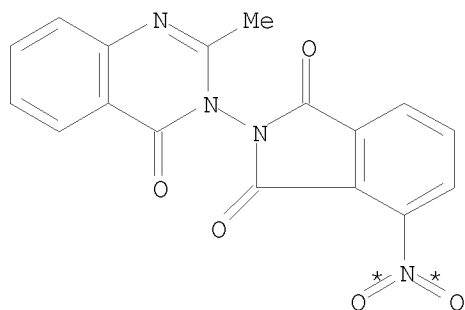
STAGE(2)

RCT AE 22185-75-7  
RGT E 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 45 minutes, 0 - 5 deg C  
SUBSTAGE(2) 24 hours, 0 - 5 deg C, pH 5 - 6

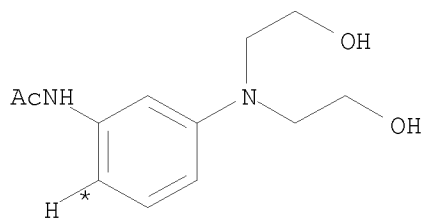
PRO AF 500226-03-9

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RX(22) OF 29 COMPOSED OF RX(15), RX(7)  
RX(22) AG + Q ==> R



AG



Q

2  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(15) RCT AG 500226-04-0

STAGE(1)

RGT E 7647-01-0 HCl, AH 7439-89-6 Fe  
SOL 67-56-1 MeOH, 7732-18-5 Water  
CON SUBSTAGE(1) 1 hour, reflux  
SUBSTAGE(2) 2 hours, reflux

STAGE(2)

RGT AI 7664-41-7 NH3  
SOL 7732-18-5 Water

PRO A 500226-05-1

RX(7) RCT A 500226-05-1

STAGE(1)

RGT D 7632-00-0 NaNO2, E 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 0 - 5 deg C

STAGE(2)

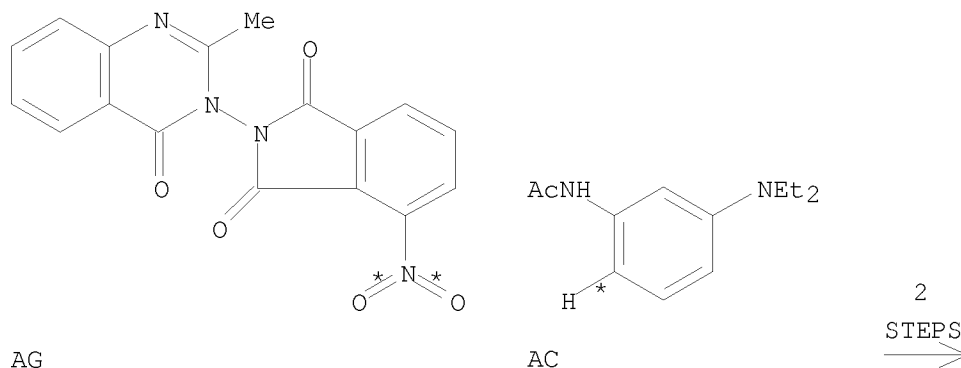
RCT Q 92-02-4  
RGT E 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 45 minutes, 0 - 5 deg C  
SUBSTAGE(2) 24 hours, 0 - 5 deg C, pH 5 - 6

PRO R 500225-96-7

RX(28) OF 29 COMPOSED OF RX(15), RX(13)

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RX(28) AG + AC ==> AD



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(15) RCT AG 500226-04-0

STAGE(1)

RGT E 7647-01-0 HCl, AH 7439-89-6 Fe

SOL 67-56-1 MeOH, 7732-18-5 Water

CON SUBSTAGE(1) 1 hour, reflux

SUBSTAGE(2) 2 hours, reflux

STAGE(2)

RGT AI 7664-41-7 NH3

SOL 7732-18-5 Water

PRO A 500226-05-1

RX(13) RCT A 500226-05-1

STAGE(1)

RGT D 7632-00-0 NaNO2, E 7647-01-0 HCl

SOL 7732-18-5 Water

CON 0 - 5 deg C

STAGE(2)

RCT AC 6375-46-8

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

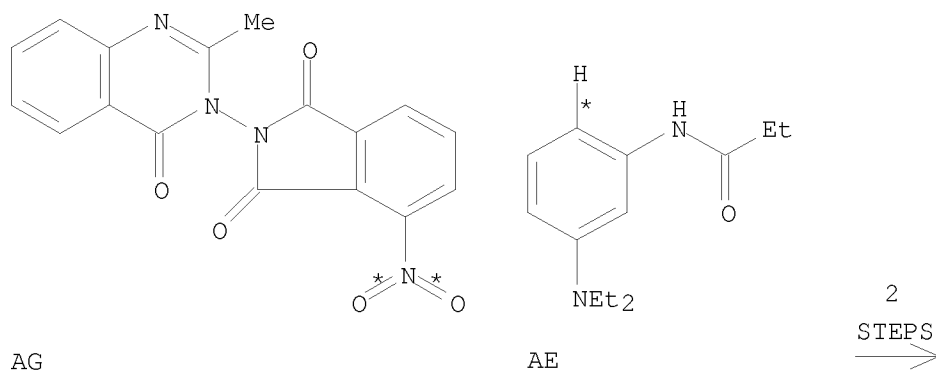
CON SUBSTAGE(1) 45 minutes, 0 - 5 deg C

SUBSTAGE(2) 24 hours, 0 - 5 deg C, pH 5 - 6

PRO AD 500226-02-8

RX(29) OF 29 COMPOSED OF RX(15), RX(14)

RX(29) AG + AE ==> AF



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(15) RCT AG 500226-04-0

STAGE(1)

RGT E 7647-01-0 HCl, AH 7439-89-6 Fe  
SOL 67-56-1 MeOH, 7732-18-5 Water  
CON SUBSTAGE(1) 1 hour, reflux  
SUBSTAGE(2) 2 hours, reflux

STAGE(2)

RGT AI 7664-41-7 NH3  
SOL 7732-18-5 Water

PRO A 500226-05-1

RX(14) RCT A 500226-05-1

STAGE(1)

RGT D 7632-00-0 NaNO2, E 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 0 - 5 deg C

STAGE(2)

RCT AE 22185-75-7  
RGT E 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 45 minutes, 0 - 5 deg C  
SUBSTAGE(2) 24 hours, 0 - 5 deg C, pH 5 - 6

PRO AF 500226-03-9

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 93 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 138:122608 CASREACT

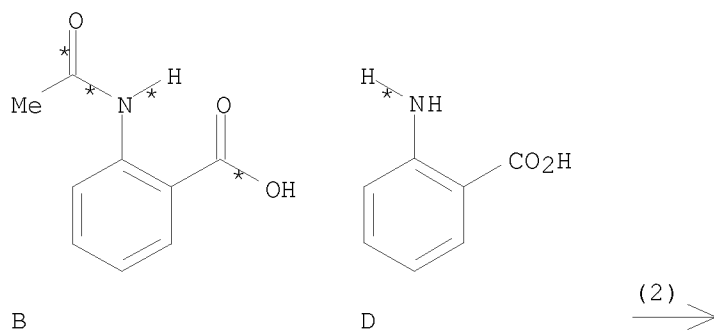
TITLE: Synthesis of derivatives of 4(3H)-quinazolinone with biological activities from N-acetylanthranilic acid



AUTHOR(S): Nguyen, Ngoc Ninh; Truong, The Ky  
 CORPORATE SOURCE: Institute of Testing, Ho Chi Minh City, Vietnam  
 SOURCE: Tap Chi Duoc Hoc (2002), (1), 19-22  
 CODEN: TCDHDQ; ISSN: 0258-6967  
 PUBLISHER: Bo Y Te Xuat Ban  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Vietnamese

AB 4(3H)-Quinazolinone derivs. were synthesized by the condensation of N-acetylthranilic acid with aromatic amines or heteroarom. amines, resp. The obtained compds. were characterized by their m.p., elemental anal. data, and their mass, UV, IR, <sup>1</sup>H and <sup>13</sup>C NMR spectra. The obtained derivs. of 4(3H)-quinazolinone were also biol. screened for hypnotic, analgesic, antibacterial and cytotoxic activities. 3-(2-Hydroxy-3-pyridinyl)-2-methyl-4(3H)-quinazolinone at 25 mg/kg showed analgesic activity in mice. No compds. showed hypnotic, cytotoxic and antibacterial activity.

RX(2) OF 15 ...B + D ==> E



E  
 YIELD 62%

RX(2) RCT B 89-52-1, D 118-92-3

STAGE(1)

CON SUBSTAGE(1) 20 minutes, 150 - 160 deg C  
 SUBSTAGE(2) 90 minutes, 160 deg C  
 SUBSTAGE(3) 160 deg C -> 120 deg C

STAGE(2)

RGT C 7732-18-5 Water

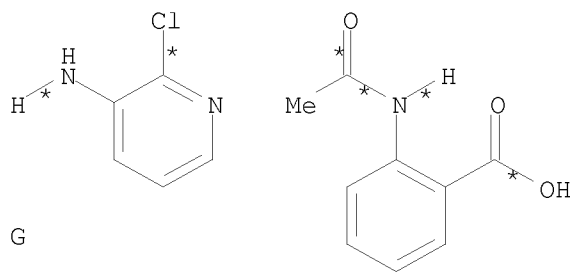
10/ 562,112

CON 120 deg C

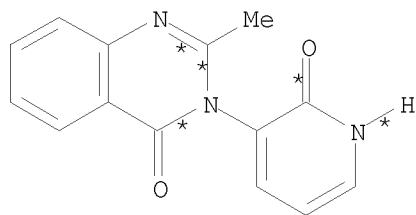
PRO E 4005-06-5

NTE polyphosphoric acid used as solvent

RX(4) OF 15 ...G + B ==> H



(4)  $\longrightarrow$



H  
YIELD 41%

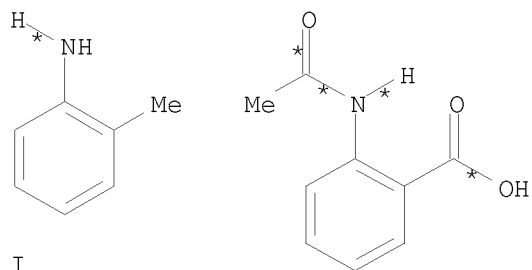
RX(4) RCT G 6298-19-7, B 89-52-1

PRO H 88369-51-1

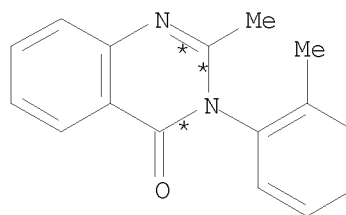
CON 180 deg C

NTE polyphosphoric acid used as solvent

RX(5) OF 15 ...I + B ==> J



(5)  $\longrightarrow$



J  
YIELD 56%

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RX(5) RCT I 95-53-4, B 89-52-1

STAGE(1)

CON SUBSTAGE(1) 20 minutes, 150 - 160 deg C

SUBSTAGE(2) 90 minutes, 160 deg C

SUBSTAGE(3) 160 deg C -> 120 deg C

STAGE(2)

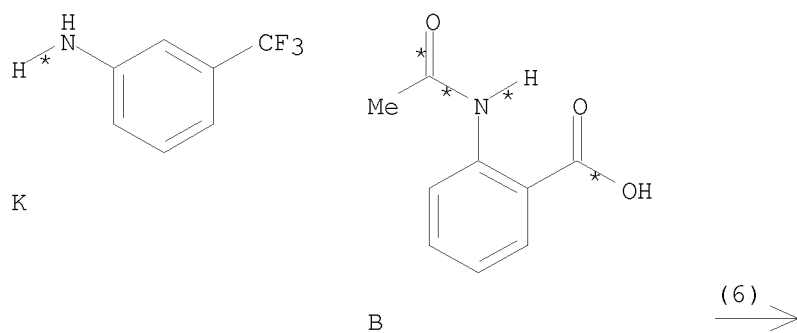
RGT C 7732-18-5 Water

CON 120 deg C

PRO J 72-44-6

NTE polyphosphoric acid used as solvent

RX(6) OF 15 ...K + B ==> L



L  
YIELD 73%

RX(6) RCT K 98-16-8, B 89-52-1

STAGE(1)

CON SUBSTAGE(1) 20 minutes, 150 - 160 deg C

SUBSTAGE(2) 90 minutes, 160 deg C

SUBSTAGE(3) 160 deg C -> 120 deg C

STAGE(2)

RGT C 7732-18-5 Water

CON 120 deg C

PRO L 1788-98-3

NTE polyphosphoric acid used as solvent

L3 ANSWER 94 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 138:14040 CASREACT

TITLE: Oxidation of 3-aminoquinazolinones with lead tetraacetate. A novel synthesis of naphtho-fused azirino-pyrazolo- and 1,4,5-oxadiazepinoquinazolinones

AUTHOR(S): El-Sharief, A. M. Sh.; Ammar, Y. A.; Zahran, M. A.; Ali, A. H.

CORPORATE SOURCE: Chemistry Department, Faculty of Science, Al-Azhar University, Cairo, Egypt

SOURCE: Journal of Chemical Research, Synopses (2002), (5), 205-208

CODEN: JRPSDC; ISSN: 0308-2342

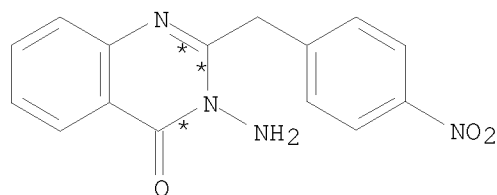
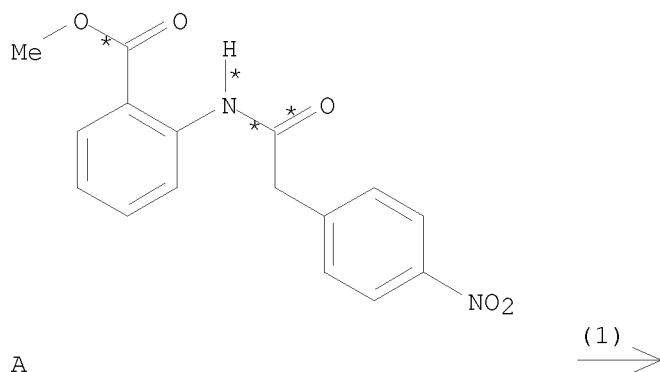
PUBLISHER: Science Reviews

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Oxidation of a 2-(arylmethyl)-3-Amino-4(3H)-quinazolinone derivs. using lead tetraacetate in methylene chloride at -20°C gave aziridine derivs. Oxidation of 2-(arylmethyl)-3-amino-4(3H)-quinazolinones gave aziridine derivs. Oxidation of 2-[(aryloxy)methyl]-3-amino-4(3H)-quinazolinones with lead tetraacetate under similar conditions gave the oxadiazepine derivs. 7H-naphtho[2',1':6,7][1,4,5]oxadiazepino[3,4-b]quinazolin-9(15H)-one and 16H-naphtho[1',2':6,7][1,4,5]oxadiazepino[3,4-b]quinazolin-14(8H)-one, resp.

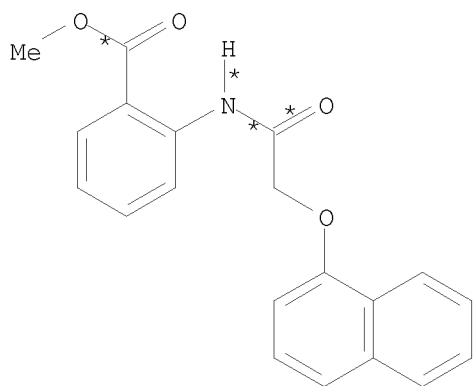
RX(1) OF 26 A ==&gt; B



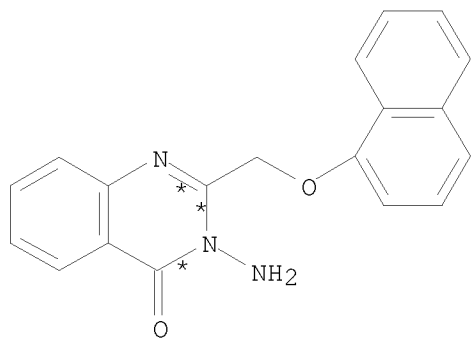
10/ 562,112

RX(1)      RCT    A 349410-48-6  
             RGT    C 302-01-2 N2H4  
             PRO    B 258524-94-6  
             SOL    71-36-3 BuOH  
             CON    4 - 6 hours, reflux

RX(8) OF 26      Q ==> R...



Q

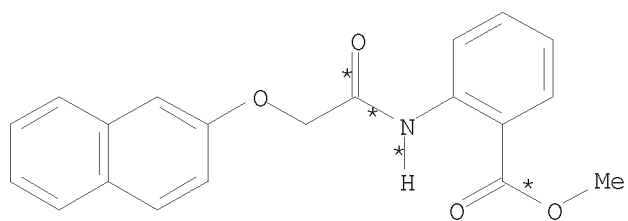


R

RX(8)      RCT    Q 420824-23-3  
             RGT    C 302-01-2 N2H4  
             PRO    R 477782-43-7  
             SOL    71-36-3 BuOH  
             CON    4 - 6 hours, reflux

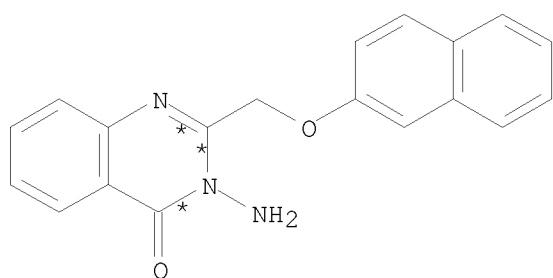
RX(9) OF 26      S ==> T...

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S

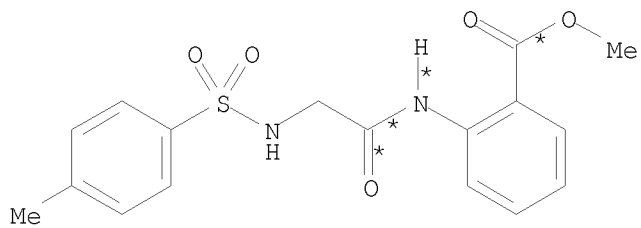
(9)  $\Rightarrow$



T

RX(9)      RCT   S 424800-39-5  
              RGT   C 302-01-2 N2H4  
              PRO   T 123798-73-2  
              SOL   71-36-3 BuOH  
              CON   4 - 6 hours, reflux

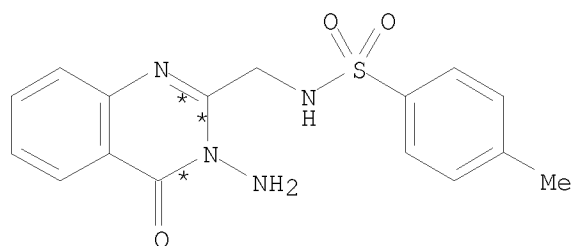
RX(12) OF 26      W    $\Rightarrow$    X...



W

(12)  $\Rightarrow$

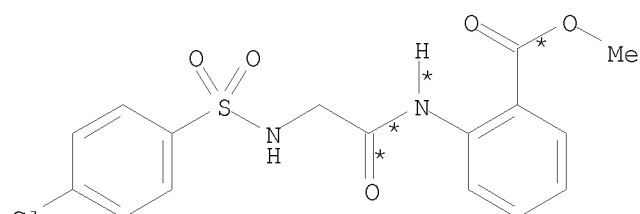
10/ 562,112



X

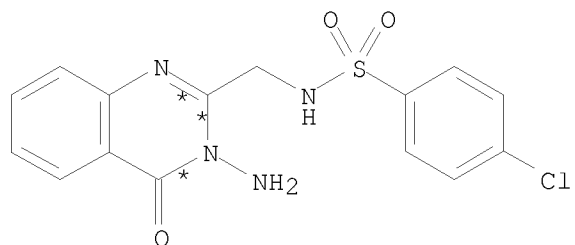
RX(12)      RCT    W 219970-85-1  
              RGT    C 302-01-2 N<sub>2</sub>H<sub>4</sub>  
              PRO    X 219970-93-1  
              SOL    71-36-3 BuOH  
              CON    4 - 6 hours, reflux

RX(13) OF 26      Y    ==>    Z...



Y

(13)

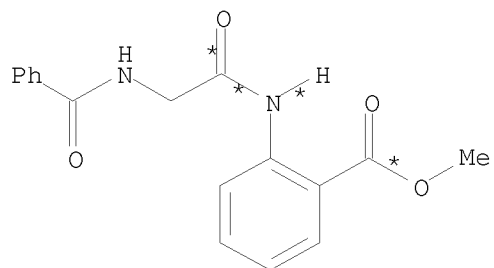


Z

RX(13)      RCT    Y 219970-86-2  
              RGT    C 302-01-2 N<sub>2</sub>H<sub>4</sub>  
              PRO    Z 219970-94-2  
              SOL    71-36-3 BuOH  
              CON    4 - 6 hours, reflux

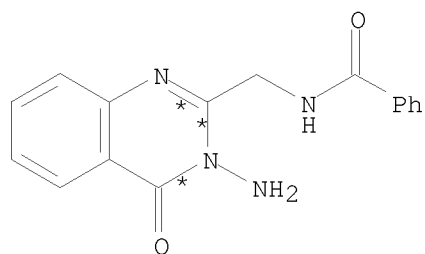
RX(14) OF 26      AA    ==>    AB...

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AA

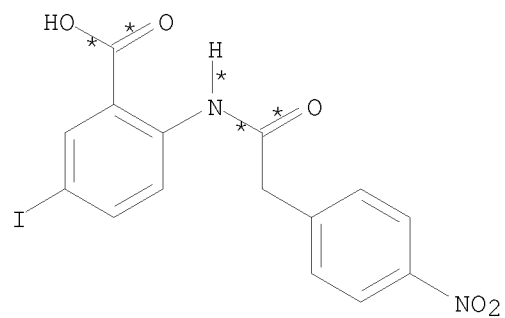
(14)



AB

RX(14)     RCT    AA 219970-89-5  
             RGT    C 302-01-2 N<sub>2</sub>H<sub>4</sub>  
             PRO    AB 219970-96-4  
             SOL    71-36-3 BuOH  
             CON    4 - 6 hours, reflux

RX(18) OF 26 COMPOSED OF RX(2), RX(4)  
RX(18)     E     ==>    J

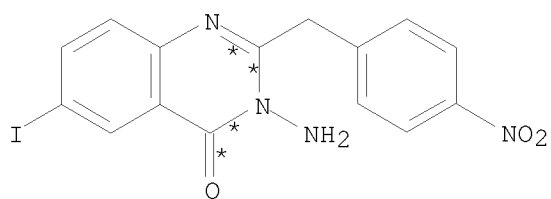


E

2  
STEPS



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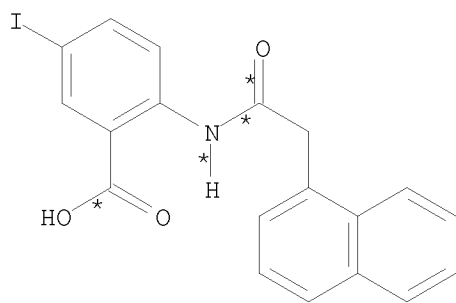


J

RX(2)      RCT   E 477782-35-7  
             PRO   F 477782-37-9  
             SOL   108-24-7 Ac2O

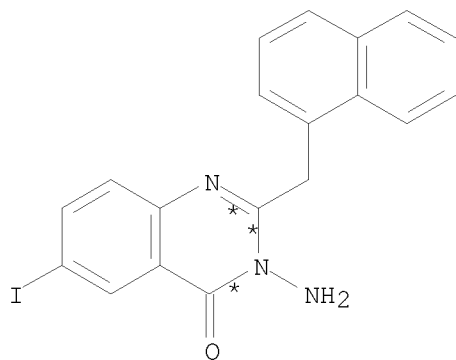
RX(4)      RCT   F 477782-37-9  
             RGT   C 302-01-2 N2H4  
             PRO   J 477782-39-1  
             SOL   71-36-3 BuOH  
             CON   4 - 6 hours, reflux

RX(19) OF 26 COMPOSED OF RX(3), RX(5)  
RX(19)      H   ==>   K



H

2  
STEPS  
→



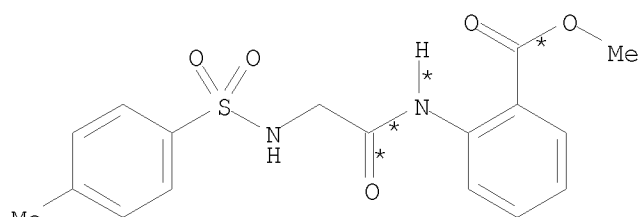
K

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RX(3)      RCT    H 477782-36-8  
             PRO    I 477782-38-0  
             SOL    108-24-7 Ac2O

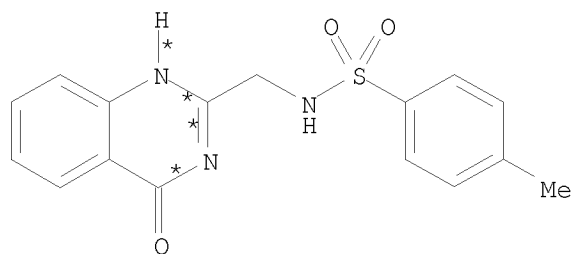
RX(5)      RCT    I 477782-38-0  
             RGT    C 302-01-2 N2H4  
             PRO    K 477782-40-4  
             SOL    71-36-3 BuOH  
             CON    4 - 6 hours, reflux

RX(23) OF 26 COMPOSED OF RX(12), RX(15)  
RX(23)      W    ==>    AC



W

2  
STEPS  
→



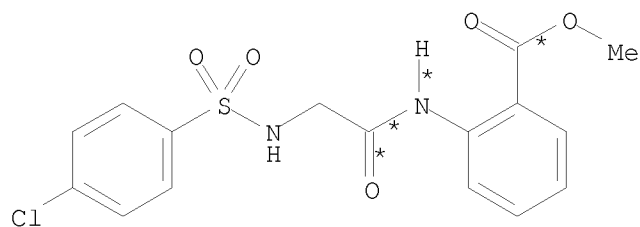
AC

RX(12)      RCT    W 219970-85-1  
             RGT    C 302-01-2 N2H4  
             PRO    X 219970-93-1  
             SOL    71-36-3 BuOH  
             CON    4 - 6 hours, reflux

RX(15)      RCT    X 219970-93-1  
             RGT    M 546-67-8 Pb(OAc)<sub>4</sub>  
             PRO    AC 219971-11-6  
             SOL    75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
             CON    -20 deg C

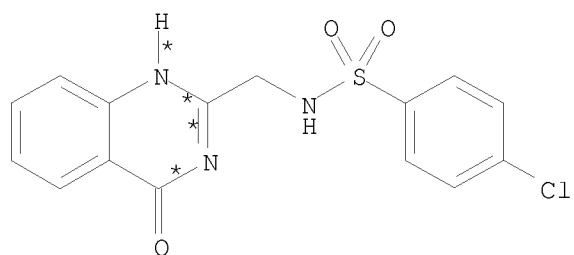
RX(24) OF 26 COMPOSED OF RX(13), RX(16)  
RX(24)      Y    ==>    AD

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Y

2  
STEPS  
→

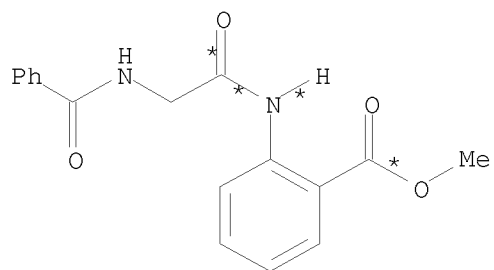


AD

RX(13)      RCT    Y 219970-86-2  
               RGT    C 302-01-2 N2H4  
               PRO    Z 219970-94-2  
               SOL    71-36-3 BuOH  
               CON    4 - 6 hours, reflux

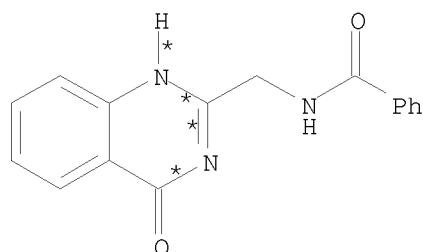
RX(16)      RCT    Z 219970-94-2  
               RGT    M 546-67-8 Pb(OAc)4  
               PRO    AD 219971-12-7  
               SOL    75-09-2 CH2Cl2  
               CON    -20 deg C

RX(25) OF 26 COMPOSED OF RX(14), RX(17)  
 RX(25)      AA ==> AE



AA

2  
STEPS  
→



AE

RX(14) RCT AA 219970-89-5  
 RGT C 302-01-2 N<sub>2</sub>H<sub>4</sub>  
 PRO AB 219970-96-4  
 SOL 71-36-3 BuOH  
 CON 4 - 6 hours, reflux

RX(17) RCT AB 219970-96-4  
 RGT M 546-67-8 Pb(OAc)<sub>4</sub>  
 PRO AE 219971-22-9  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON -20 deg C

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 95 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 137:279208 CASREACT

TITLE: Preparation of (indazol-5-ylamino)quinazolines as  
 Rho-kinase inhibitors

INVENTOR(S): Nagarathnam, Dhanapalan; Asgari, Davoud; Shao,  
 Jianxing; Liu, Xiao-Gao; Khire, Uday; Wang, Chunguang;  
 Hart, Barry; Boyer, Stephen; Weber, Olaf; Lynch, Mark;  
 Bankston, Donald

PATENT ASSIGNEE(S): Bayer Corporation, USA

SOURCE: PCT Int. Appl., 74 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002076976	A2	20021003	WO 2002-US8659	20020322
WO 2002076976	A3	20021212		

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 CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,  
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,  
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,  
 PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,  
 US, UZ, VN, YU, ZA, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,

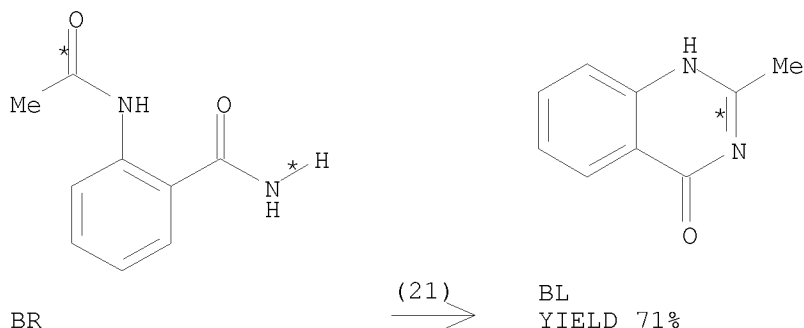
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CA	2441492	A1	20021003	CA	2002-2441492	20020322
AU	2002250394	A1	20021008	AU	2002-250394	20020322
US	20030125344	A1	20030703	US	2002-103566	20020322
EP	1370553	A2	20031217	EP	2002-719303	20020322
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JP	2004524350	T	20040812	JP	2002-576234	20020322
AT	325795	T	20060615	AT	2002-719303	20020322
TW	261055	B	20060901	TW	2002-91105591	20020322
PT	1370553	T	20060929	PT	2002-719303	20020322
ES	2264477	T3	20070101	ES	2002-719303	20020322
US	20030220357	A1	20031127	US	2002-252369	20020924
CA	2507381	A1	20040408	CA	2003-2507381	20030924
WO	2004029045	A2	20040408	WO	2003-US29538	20030924
WO	2004029045	A3	20040722			
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AU	2003270785	A1	20040419	AU	2003-270785	20030924
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EP	1542992	A2	20050622	EP	2003-752497	20030924
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JP	2006508068	T	20060309	JP	2004-540124	20030924
EP	1953152	A1	20080806	EP	2008-103780	20030924
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HK	1061030	A1	20060908	HK	2004-104115	20040609
MX	2005003273	A	20051018	MX	2005-3273	20050323
US	20060142313	A1	20060629	US	2006-354977	20060216
US	20060142314	A1	20060629	US	2006-354978	20060216
PRIORITY APPLN. INFO.:				US	2001-277974P	20010323
				US	2001-315341P	20010829
				US	2001-315338P	20010829
				US	2002-103565	20020322
				US	2002-103566	20020322
				WO	2002-US8659	20020322
				US	2002-252369	20020924
				EP	2003-752497	20030924
				WO	2003-US29538	20030924
OTHER SOURCE(S):		MARPAT	137:279208			
GI						

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [Y = N, CR17; X = alkyl, alkoxy, thioalkoxy, amido, etc.; p = 0-3; a, c = CR5, NR6, etc.; b = CR5, N; A = H, halo, carboxy, cyano,

alkoxy, etc.; B = (un)substituted up to 3 times in any position by R5; R1,6 = H, alkyl; R2-5 = H, alkyl, alkenyl; R17 = H, alkyl, CN with provisions] were prepared For instance, 2,4-Dichloroquinazoline (preparation given) was reacted with 5-aminoindazole (THF/H2O, KOAc) to give 2-(N-(1H-indazol-5-yl)amino)-4-chloroquinazoline in 92% yield. This was coupled to 2,4-dichlorophenylboronic acid (ethylene glycol di-Me ether, Pd(dppf)Cl2, NaHCO3, reflux) to give II. I are rho-kinase inhibitors and are useful for inhibiting tumor growth, treating erectile dysfunction and coronary heart disease.

RX(21) OF 174 ...BR ==> BL...



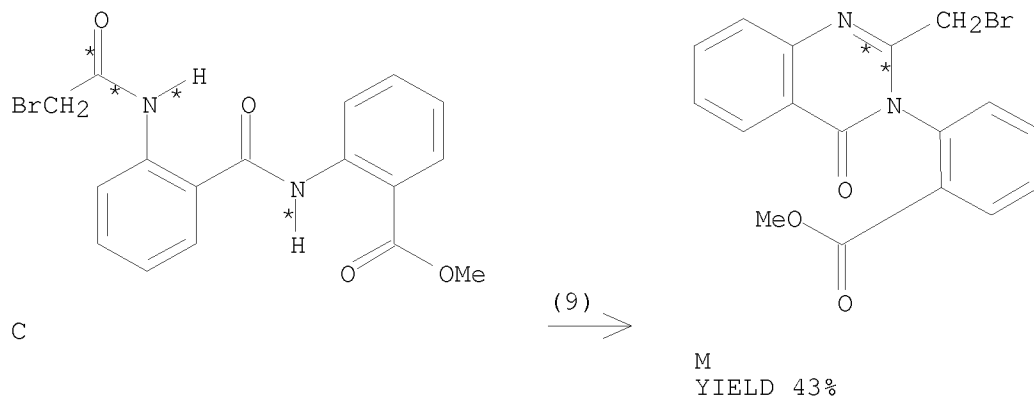
RX(21) RCT BR 33809-77-7  
RGT AF 1310-73-2 NaOH  
PRO BL 1769-24-0  
SOL 7732-18-5 Water, 64-17-5 EtOH

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 96 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 137:247841 CASREACT  
TITLE: Oxygen analogs of the benzodiazepine alkaloids sclerotigenin and circumdatin F  
AUTHOR(S): Witt, Anette; Bergman, Jan  
CORPORATE SOURCE: Unit for Organic Chemistry, Department of Biosciences, Novum Research Park, Karolinska Institute and Sodertorn University College, Huddinge, SE-141 57, Swed.  
SOURCE: Journal of Heterocyclic Chemistry (2002), 39(2), 351-355  
CODEN: JHTCAD; ISSN: 0022-152X  
PUBLISHER: HeteroCorporation  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB A new type of fused oxazepinones, which are analogs of sclerotigenin and circumdatin F, were obtained in a two step synthesis from 2-(2-amino-benzoylamino)benzoic acid or the corresponding Me ester. Secondly a new synthesis of circumdatin F arose from this work, where 2-(2-propionylaminobenzoylamino)benzoic acid Me ester was used as an intermediate.

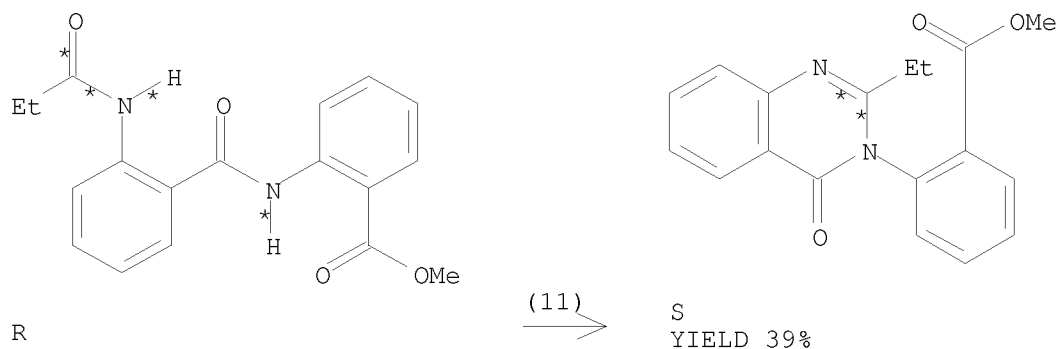
10/ 562,112

RX(9) OF 29      ...C ==> M...



RX(9)      RCT    C 460062-20-8  
             PRO    M 61554-52-7  
             CAT    104-15-4 TsOH  
             SOL    108-88-3 PhMe  
             CON    60 hours, reflux

RX(11) OF 29      ...R ==> S...



RX(11)      RCT    R 460062-44-6

             STAGE(1)  
             SOL    68-12-2 DMF  
             CON    65 hours, reflux

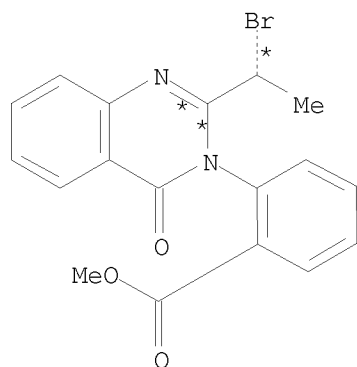
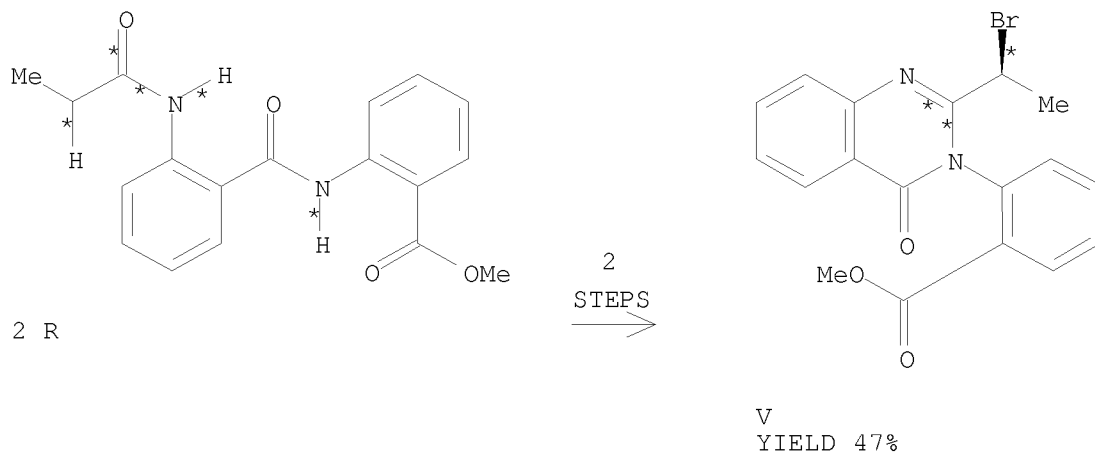
             STAGE(2)  
             RGT    U 7732-18-5 Water  
             CON    1 hour

             PRO    S 94209-49-1

RX(23) OF 29 COMPOSED OF RX(11), RX(12)

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RX(23)      2 R    ==>   V   +   W



RX(11)      RCT   R 460062-44-6

STAGE(1)

SOL   68-12-2 DMF

CON   65 hours, reflux

STAGE(2)

RGT   U 7732-18-5 Water

CON   1 hour

PRO   S 94209-49-1

RX(12)

RCT   S 94209-49-1

RGT   X 127-09-3 AcONa, Y 7726-95-6 Br<sub>2</sub>

PRO   V 460062-47-9, W 460062-48-0

SOL   7732-18-5 Water, 64-19-7 AcOH

CON   SUBSTAGE(1) 15 minutes, 60 deg C

      SUBSTAGE(2) 1.5 hours

NTE   stereoselective, overall yield of distereomeric mixture = 87%



and ratio is 7:3

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 97 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 137:185777 CASREACT

TITLE: Synthesis and In Vitro Antitumor Activity of Thiophene Analogues of 5-Chloro-5,8-dideazafolic Acid and 2-Methyl-2-desamino-5-chloro-5,8-dideazafolic Acid

AUTHOR(S): Forsch, Ronald A.; Wright, Joel E.; Rosowsky, Andre

CORPORATE SOURCE: Dana-Farber Cancer Institute and the Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA

SOURCE: Bioorganic & Medicinal Chemistry (2002), 10(6), 2067-2076

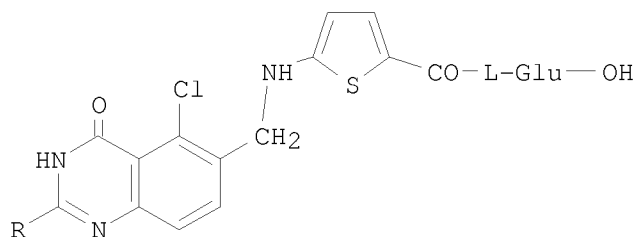
CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

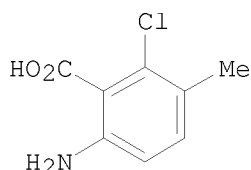
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

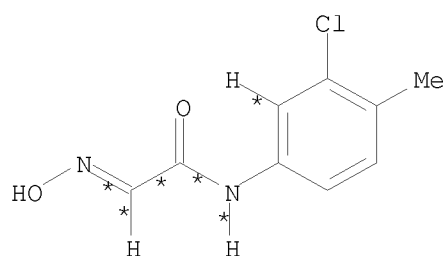


III

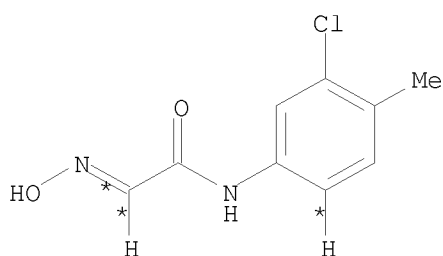
AB N-[5-[N-(2-Amino-5-chloro-3,4-dihydro-4-oxoquinazolin-6-yl)methylamino]-2-thenoyl]-L-glutamic acid (I; R = NH<sub>2</sub>) and N-[5-[N-(5-chloro-3,4-dihydro-2-methyl-4-oxoquinazolin-6-yl)methylamino]-2-thenoyl]-L-glutamic acid (I; R = Me), the first reported thiophene analogs of 5-chloro-5,8-dideazafolic acid, were synthesized and tested as inhibitors of tumor cell growth in culture. 4-Chloro-5-methylisatin was converted stepwise to Me 2-amino-5-methyl-6-chlorobenzoate and 2-amino-5-chloro-3,4-dihydro-6-methyl-4-oxoquinazoline. Pivaloylation of the 2-amino group, followed by NBS bromination, condensation with di-tert-Bu N-(5-amino-2-thenoyl)-L-glutamate (II), and stepwise cleavage of the protecting groups with ammonia and TFA yielded I (R = NH<sub>2</sub>). Treatment of (III) with acetic anhydride afforded 2,6-dimethyl-5-chlorobenz[1,3-d]oxazin-4-one, which on reaction with ammonia, NaOH was converted to 2,6-dimethyl-5-chloro-3,4-dihydroquinazolin-4-one (IV). Bromination of IV, followed by condensation with 28 and ester cleavage with TFA, yielded I (R = Me). The IC<sub>50</sub> of I (R = NH<sub>2</sub> or Me) against CCRF-CEM human leukemic lymphoblasts was 1.8±0.1 and 2.1±0.8 μM, resp.

RX(53) OF 209 COMPOSED OF RX(3), RX(6), RX(8), RX(18)

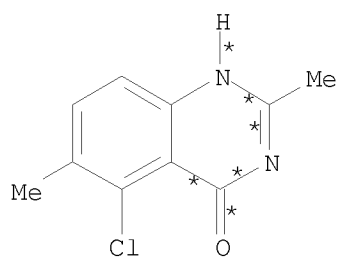
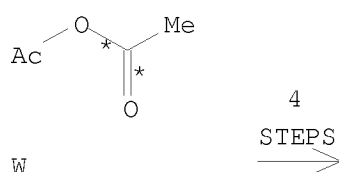
RX(53) 2 I + W ==> BC



I



I



BC  
YIELD 99%

RX(3) RCT I 155184-79-5

STAGE (1)

RGT N 7664-93-9 H2SO4

STAGE (2)

SOL 67-64-1 Me2CO

PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2

STAGE (1)

RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2

SOL 7732-18-5 Water

STAGE (2)

RGT S 7647-01-0 HCl

SOL 7732-18-5 Water

PRO P 155184-82-0

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RX(8) RCT P 155184-82-0, W 108-24-7  
PRO X 450407-91-7  
SOL 108-24-7 Ac2O

RX(18) RCT X 450407-91-7

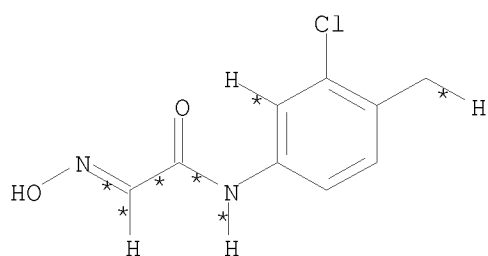
STAGE(1)  
RGT BB 7664-41-7 NH3

STAGE(2)  
RGT Q 1310-73-2 NaOH  
SOL 7732-18-5 Water

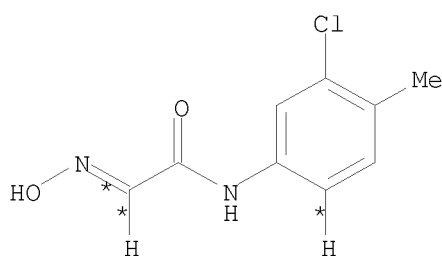
STAGE(3)  
RGT O 64-19-7 AcOH

PRO BC 450407-92-8

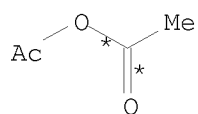
RX(93) OF 209 COMPOSED OF RX(3), RX(6), RX(8), RX(18), RX(19)  
RX(93) 2 I + W ==> BD



I

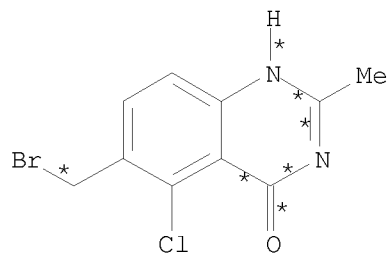


I



W

5  
STEPS  
→



BD  
YIELD 77%

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RX(3) RCT I 155184-79-5

STAGE(1)

RGT N 7664-93-9 H2SO4

STAGE(2)

SOL 67-64-1 Me2CO

PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2

STAGE(1)

RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2

SOL 7732-18-5 Water

STAGE(2)

RGT S 7647-01-0 HCl

SOL 7732-18-5 Water

PRO P 155184-82-0

RX(8) RCT P 155184-82-0, W 108-24-7

PRO X 450407-91-7

SOL 108-24-7 Ac2O

RX(18) RCT X 450407-91-7

STAGE(1)

RGT BB 7664-41-7 NH3

STAGE(2)

RGT Q 1310-73-2 NaOH

SOL 7732-18-5 Water

STAGE(3)

RGT O 64-19-7 AcOH

PRO BC 450407-92-8

RX(19) RCT BC 450407-92-8

RGT AN 128-08-5 Bromosuccinimide

PRO BD 450407-93-9

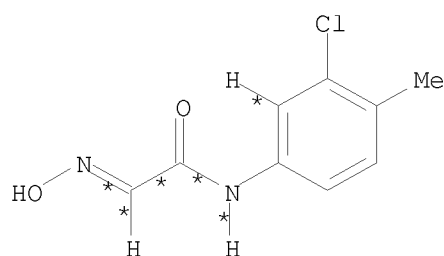
CAT 94-36-0 Benzoyl peroxide

SOL 67-66-3 CHCl3

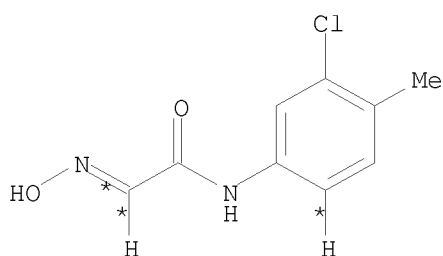
RX(99) OF 209 COMPOSED OF RX(3), RX(6), RX(8), RX(18), RX(19), RX(20)

RX(99) 2 I + W + AU ==> BE

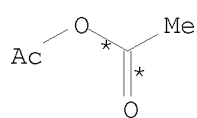
10/ 562,112



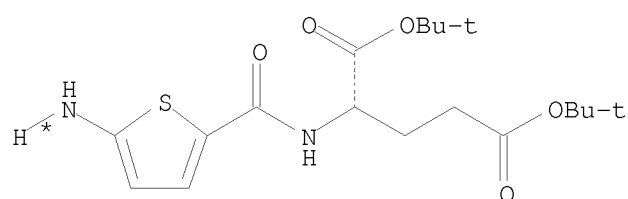
I



I

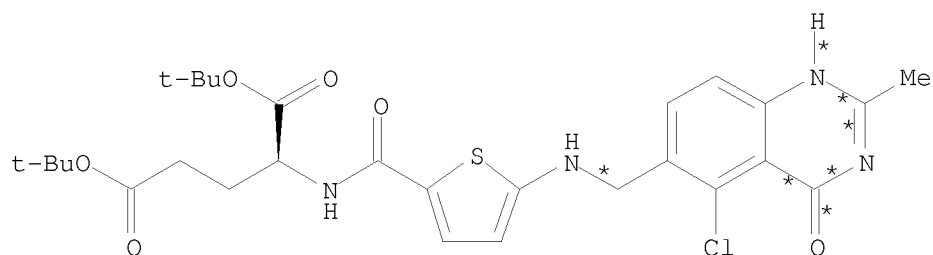


W



AU

6  
STEPS  
→



BE

RX(3) RCT I 155184-79-5

STAGE(1)

RGT N 7664-93-9 H2SO4

STAGE(2)

SOL 67-64-1 Me2CO

PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2

STAGE(1)

RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2

SOL 7732-18-5 Water

STAGE(2)

RGT S 7647-01-0 HCl

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SOL 7732-18-5 Water

PRO P 155184-82-0

RX(8) RCT P 155184-82-0, W 108-24-7  
PRO X 450407-91-7  
SOL 108-24-7 Ac2O

RX(18) RCT X 450407-91-7

STAGE(1)

RGT BB 7664-41-7 NH3

STAGE(2)

RGT Q 1310-73-2 NaOH

SOL 7732-18-5 Water

STAGE(3)

RGT O 64-19-7 AcOH

PRO BC 450407-92-8

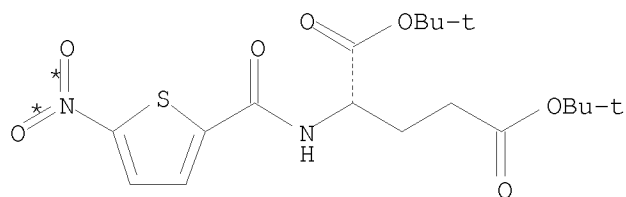
RX(19) RCT BC 450407-92-8  
RGT AN 128-08-5 Bromosuccinimide  
PRO BD 450407-93-9  
CAT 94-36-0 Benzoyl peroxide  
SOL 67-66-3 CHCl3

RX(20) RCT BD 450407-93-9, AU 132463-36-6  
RGT AZ 144-55-8 NaHCO3  
PRO BE 450407-94-0  
SOL 68-12-2 DMF

RX(110) OF 209 COMPOSED OF REACTION SEQUENCE RX(15), RX(20)  
AND REACTION SEQUENCE RX(3), RX(6), RX(8), RX(18), RX(19),  
RX(20)

...AR ==> AU...

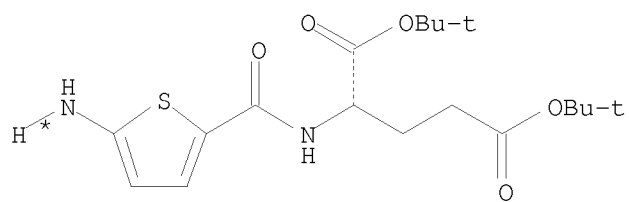
...2 I + W + AU ==> BE



AR

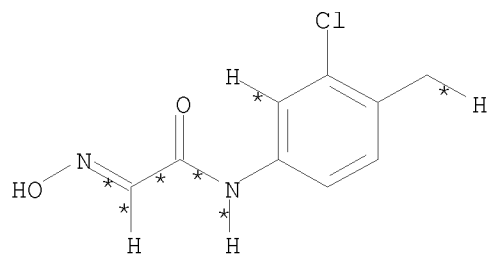
6  
STEPS  
→

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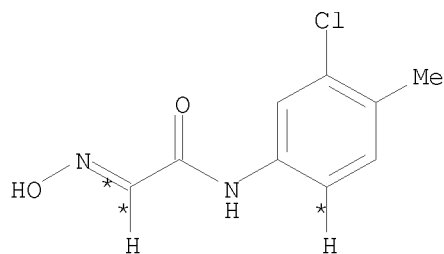


AU

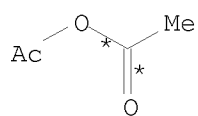
START NEXT REACTION SEQUENCE



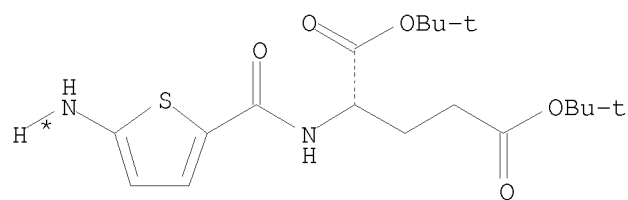
I



I

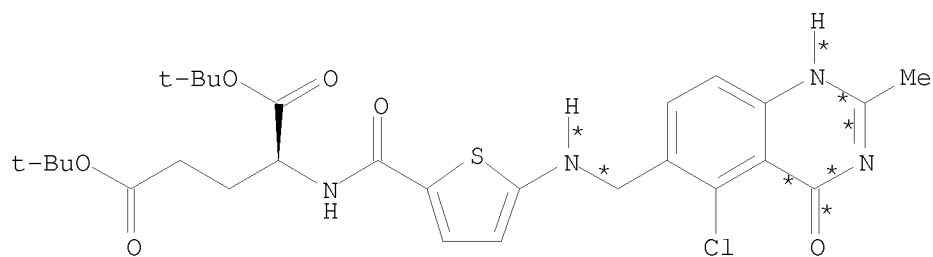


W



AU

6  
STEPS  
→



BE

RX(15)    RCT    AR 450407-87-1  
              RGT    AV 7439-89-6 Fe  
              PRO    AU 132463-36-6  
              CAT    7720-78-7 FeSO4  
              SOL    67-56-1 MeOH

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RX(3) RCT I 155184-79-5

STAGE(1)

RGT N 7664-93-9 H2SO4

STAGE(2)

SOL 67-64-1 Me2CO

PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2

STAGE(1)

RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2

SOL 7732-18-5 Water

STAGE(2)

RGT S 7647-01-0 HCl

SOL 7732-18-5 Water

PRO P 155184-82-0

RX(8) RCT P 155184-82-0, W 108-24-7

PRO X 450407-91-7

SOL 108-24-7 Ac2O

RX(18) RCT X 450407-91-7

STAGE(1)

RGT BB 7664-41-7 NH3

STAGE(2)

RGT Q 1310-73-2 NaOH

SOL 7732-18-5 Water

STAGE(3)

RGT O 64-19-7 AcOH

PRO BC 450407-92-8

RX(19) RCT BC 450407-92-8

RGT AN 128-08-5 Bromosuccinimide

PRO BD 450407-93-9

CAT 94-36-0 Benzoyl peroxide

SOL 67-66-3 CHCl3

RX(20) RCT BD 450407-93-9, AU 132463-36-6

RGT AZ 144-55-8 NaHCO3

PRO BE 450407-94-0

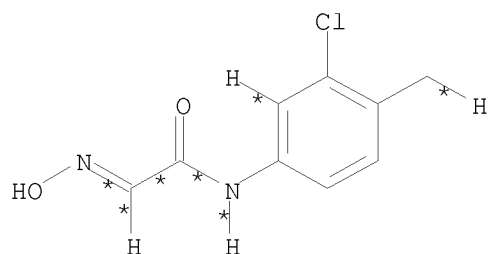
SOL 68-12-2 DMF

RX(111) OF 209 COMPOSED OF RX(3), RX(6), RX(8), RX(18), RX(19), RX(20), RX(21)

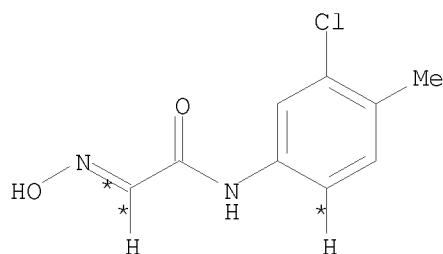
RX(111) 2 I + W + AU ==> BF



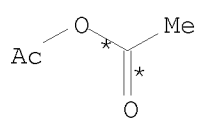
10/ 562,112



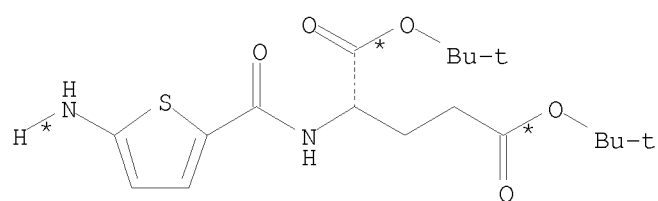
I



I

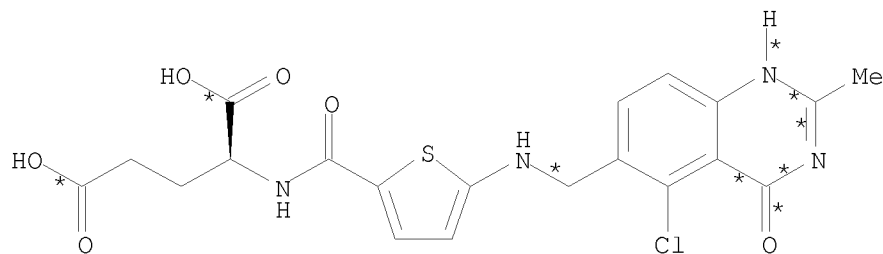


W



AU

7  
STEPS  
→



BF

YIELD 39%

RX(3) RCT I 155184-79-5

STAGE(1)

RGT N 7664-93-9 H2SO4

STAGE(2)

SOL 67-64-1 Me2CO

PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2

STAGE(1)

RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2

SOL 7732-18-5 Water

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      STAGE(2)
      RGT  S 7647-01-0 HCl
      SOL  7732-18-5 Water

PRO  P 155184-82-0

RX(8)  RCT  P 155184-82-0, W 108-24-7
      PRO  X 450407-91-7
      SOL  108-24-7 Ac2O

RX(18) RCT  X 450407-91-7

      STAGE(1)
      RGT  BB 7664-41-7 NH3

      STAGE(2)
      RGT  Q 1310-73-2 NaOH
      SOL  7732-18-5 Water

      STAGE(3)
      RGT  O 64-19-7 AcOH

PRO  BC 450407-92-8

RX(19) RCT  BC 450407-92-8
      RGT  AN 128-08-5 Bromosuccinimide
      PRO  BD 450407-93-9
      CAT  94-36-0 Benzoyl peroxide
      SOL  67-66-3 CHCl3

RX(20) RCT  BD 450407-93-9, AU 132463-36-6
      RGT  AZ 144-55-8 NaHCO3
      PRO  BE 450407-94-0
      SOL  68-12-2 DMF

RX(21) RCT  BE 450407-94-0

      STAGE(1)
      RGT  AD 76-05-1 F3CCO2H
      SOL  75-09-2 CH2Cl2

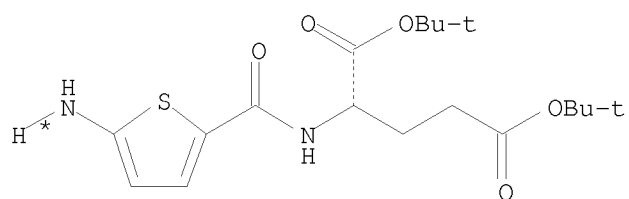
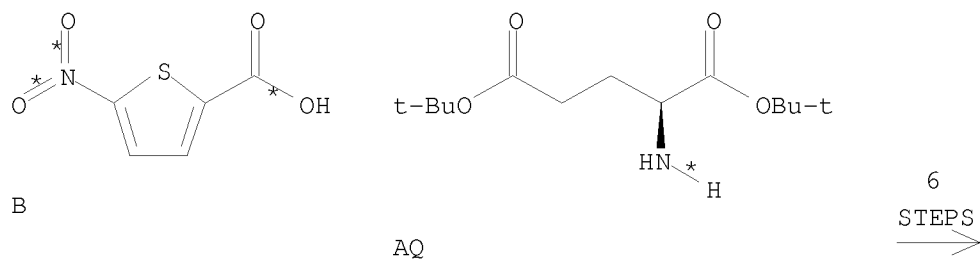
      STAGE(2)
      RGT  Q 1310-73-2 NaOH
      SOL  7732-18-5 Water

      STAGE(3)
      RGT  O 64-19-7 AcOH

PRO  BF 450407-96-2

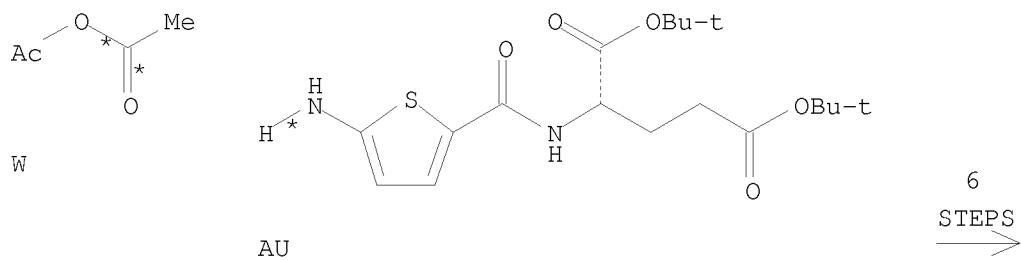
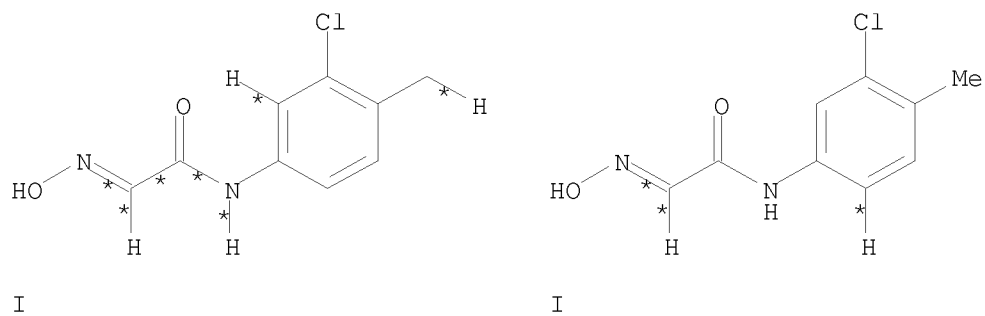
RX(158) OF 209 COMPOSED OF REACTION SEQUENCE RX(14), RX(15), RX(20)
      AND REACTION SEQUENCE RX(3), RX(6), RX(8), RX(18), RX(19),
      RX(20)
...B  +  AQ  ==>  AU...
...2 I  +  W  +  AU  ==>  BE
```

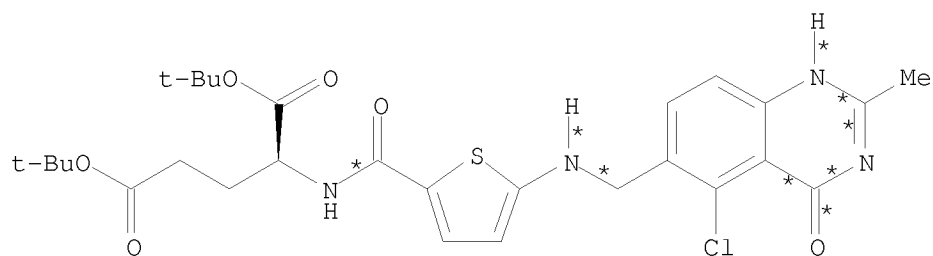
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AU

START NEXT REACTION SEQUENCE





BE

RX(14) RCT B 6317-37-9

STAGE(1)

RGT AS 7719-09-7 SOC12

STAGE(2)

RCT AQ 16874-06-9

SOL 75-09-2 CH2Cl2

STAGE(3)

RGT AK 121-44-8 Et3N

PRO AR 450407-87-1

RX(15) RCT AR 450407-87-1  
 RGT AV 7439-89-6 Fe  
 PRO AU 132463-36-6  
 CAT 7720-78-7 FeSO4  
 SOL 67-56-1 MeOH

RX(3) RCT I 155184-79-5

STAGE(1)

RGT N 7664-93-9 H2SO4

STAGE(2)

SOL 67-64-1 Me2CO

PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2

STAGE(1)

RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2

SOL 7732-18-5 Water

STAGE(2)

RGT S 7647-01-0 HCl

SOL 7732-18-5 Water

PRO P 155184-82-0

RX(8) RCT P 155184-82-0, W 108-24-7  
 PRO X 450407-91-7  
 SOL 108-24-7 Ac2O

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RX(18) RCT X 450407-91-7

STAGE(1)

RGT BB 7664-41-7 NH3

STAGE(2)

RGT Q 1310-73-2 NaOH

SOL 7732-18-5 Water

STAGE(3)

RGT O 64-19-7 AcOH

PRO BC 450407-92-8

RX(19) RCT BC 450407-92-8  
RGT AN 128-08-5 Bromosuccinimide  
PRO BD 450407-93-9  
CAT 94-36-0 Benzoyl peroxide  
SOL 67-66-3 CHCl3

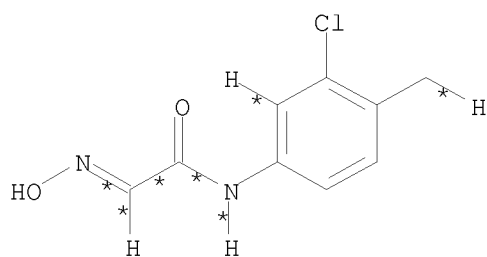
RX(20) RCT BD 450407-93-9, AU 132463-36-6  
RGT AZ 144-55-8 NaHCO3  
PRO BE 450407-94-0  
SOL 68-12-2 DMF

RX(167) OF 209 COMPOSED OF REACTION SEQUENCE RX(3), RX(6), RX(8), RX(18),  
RX(19), RX(20)

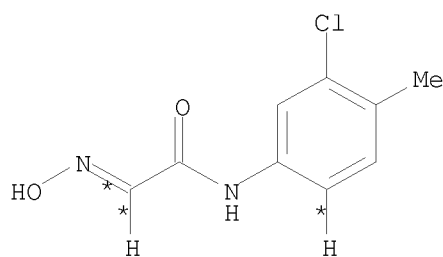
AND REACTION SEQUENCE RX(1), RX(14), RX(15), RX(20)

...2 I + W ==> BD...

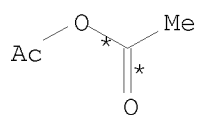
...A + AQ + BD ==> BE



I

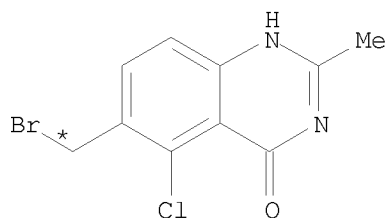


I



W

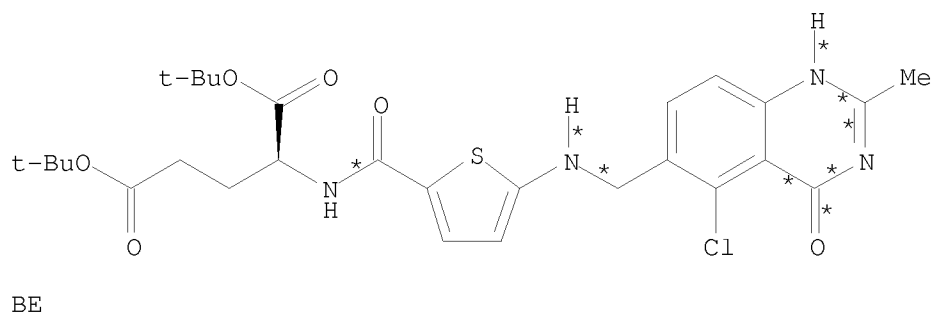
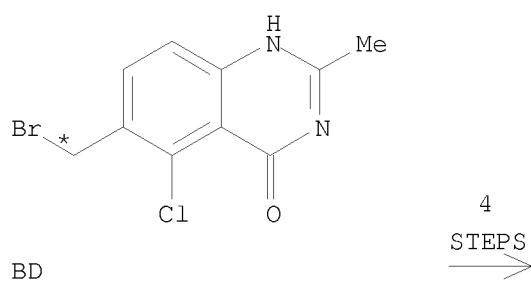
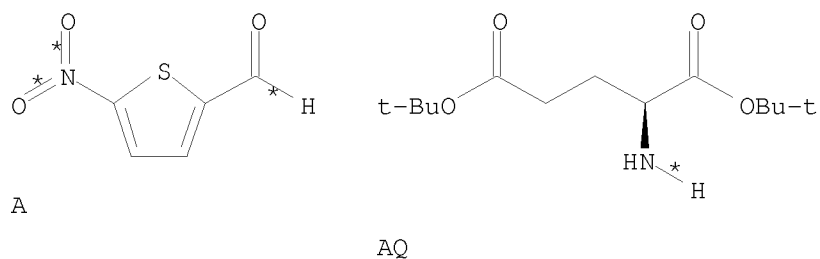
4  
STEPS  
→



BD

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START NEXT REACTION SEQUENCE



RX(3) RCT I 155184-79-5

STAGE(1)

RGT N 7664-93-9 H2SO4

STAGE(2)

SOL 67-64-1 Me2CO

PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2

STAGE(1)

RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2

SOL 7732-18-5 Water

```

          STAGE(2)
            RGT  S 7647-01-0 HCl
            SOL  7732-18-5 Water

PRO  P 155184-82-0

RX(8)  RCT  P 155184-82-0, W 108-24-7
      PRO  X 450407-91-7
      SOL  108-24-7 Ac2O

RX(18) RCT  X 450407-91-7

          STAGE(1)
            RGT  BB 7664-41-7 NH3

          STAGE(2)
            RGT  Q 1310-73-2 NaOH
            SOL  7732-18-5 Water

          STAGE(3)
            RGT  O 64-19-7 AcOH

PRO  BC 450407-92-8

RX(19) RCT  BC 450407-92-8
      RGT  AN 128-08-5 Bromosuccinimide
      PRO  BD 450407-93-9
      CAT  94-36-0 Benzoyl peroxide
      SOL  67-66-3 CHCl3

RX(1)  RCT  A 4521-33-9
      RGT  C 7722-64-7 KMnO4, D 7558-80-7 NaH2PO4
      PRO  B 6317-37-9
      SOL  7732-18-5 Water, 67-64-1 Me2CO

RX(14) RCT  B 6317-37-9

          STAGE(1)
            RGT  AS 7719-09-7 SOCl2

          STAGE(2)
            RCT  AQ 16874-06-9
            SOL  75-09-2 CH2Cl2

          STAGE(3)
            RGT  AK 121-44-8 Et3N

PRO  AR 450407-87-1

RX(15) RCT  AR 450407-87-1
      RGT  AV 7439-89-6 Fe
      PRO  AU 132463-36-6
      CAT  7720-78-7 FeSO4
      SOL  67-56-1 MeOH

RX(20) RCT  BD 450407-93-9, AU 132463-36-6
      RGT  AZ 144-55-8 NaHCO3
      PRO  BE 450407-94-0
      SOL  68-12-2 DMF

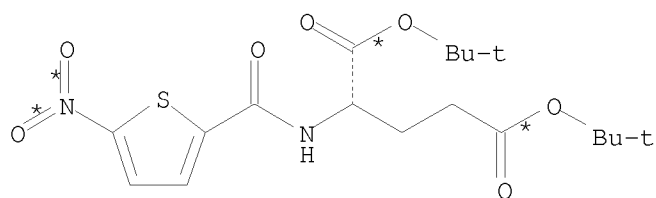
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RX(173) OF 209 COMPOSED OF REACTION SEQUENCE RX(15), RX(20), RX(21)  
AND REACTION SEQUENCE RX(3), RX(6), RX(8), RX(18), RX(19),  
RX(20), RX(21)

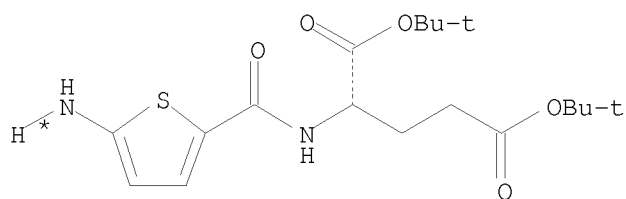
...AR ==> AU...

...2 I + W + AU ==> BF



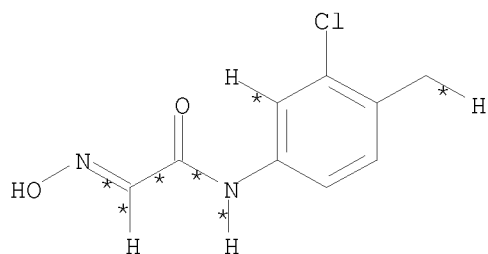
AR

7  
STEPS  
→

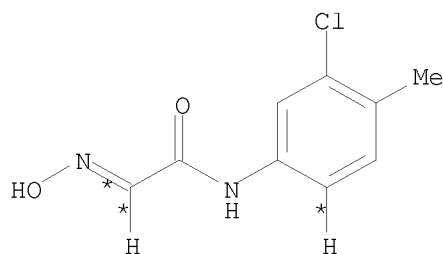


AU

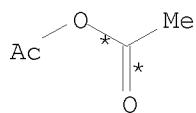
START NEXT REACTION SEQUENCE



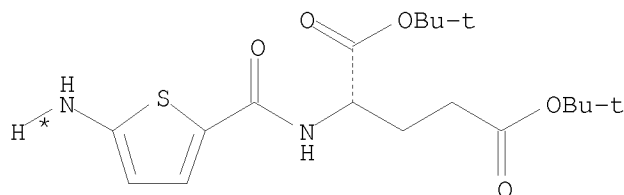
I



I



W

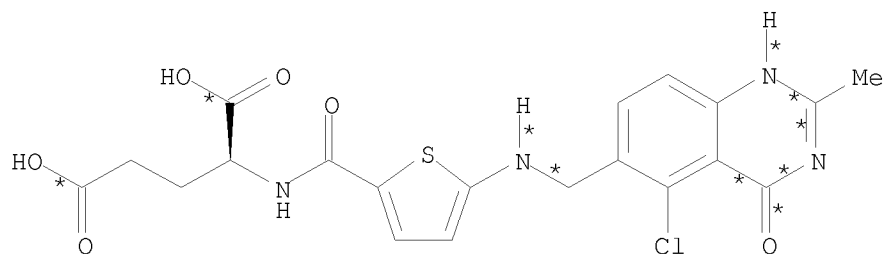


AU

7  
STEPS  
→



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BF  
YIELD 39%

RX(15) RCT AR 450407-87-1  
RGT AV 7439-89-6 Fe  
PRO AU 132463-36-6  
CAT 7720-78-7 FeSO<sub>4</sub>  
SOL 67-56-1 MeOH

RX(3) RCT I 155184-79-5  
STAGE(1)  
RGT N 7664-93-9 H<sub>2</sub>SO<sub>4</sub>

STAGE(2)  
SOL 67-64-1 Me<sub>2</sub>CO

PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2  
STAGE(1)  
RGT Q 1310-73-2 NaOH, R 7722-84-1 H<sub>2</sub>O<sub>2</sub>  
SOL 7732-18-5 Water

STAGE(2)  
RGT S 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO P 155184-82-0

RX(8) RCT P 155184-82-0, W 108-24-7  
PRO X 450407-91-7  
SOL 108-24-7 Ac<sub>2</sub>O

RX(18) RCT X 450407-91-7  
STAGE(1)  
RGT BB 7664-41-7 NH<sub>3</sub>

STAGE(2)  
RGT Q 1310-73-2 NaOH  
SOL 7732-18-5 Water

STAGE(3)  
RGT O 64-19-7 AcOH

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PRO BC 450407-92-8

RX(19) RCT BC 450407-92-8  
RGT AN 128-08-5 Bromosuccinimide  
PRO BD 450407-93-9  
CAT 94-36-0 Benzoyl peroxide  
SOL 67-66-3 CHCl<sub>3</sub>

RX(20) RCT BD 450407-93-9, AU 132463-36-6  
RGT AZ 144-55-8 NaHCO<sub>3</sub>  
PRO BE 450407-94-0  
SOL 68-12-2 DMF

RX(21) RCT BE 450407-94-0

STAGE(1)  
RGT AD 76-05-1 F<sub>3</sub>CCO<sub>2</sub>H  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

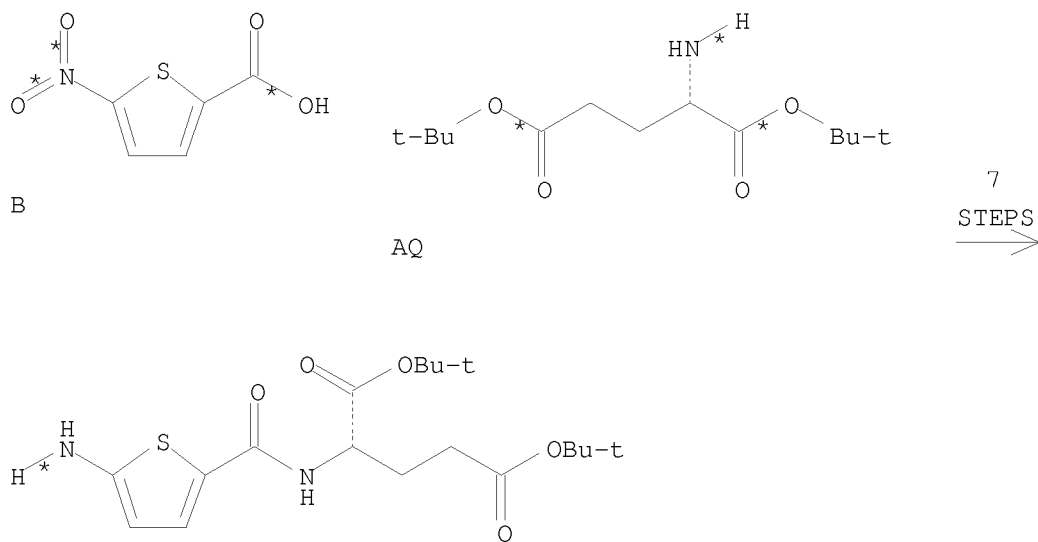
STAGE(2)  
RGT Q 1310-73-2 NaOH  
SOL 7732-18-5 Water

STAGE(3)  
RGT O 64-19-7 AcOH

PRO BF 450407-96-2

RX(174) OF 209 COMPOSED OF REACTION SEQUENCE RX(14), RX(15), RX(20), RX(21)  
AND REACTION SEQUENCE RX(3), RX(6), RX(8), RX(18), RX(19),  
RX(20), RX(21)

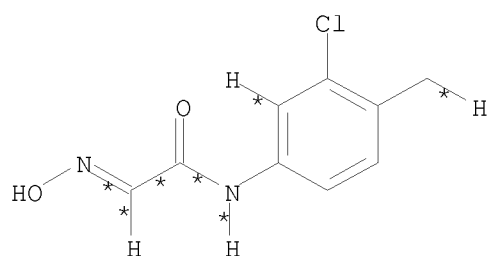
...B + AQ ==> AU...  
...2 I + W + AU ==> BF



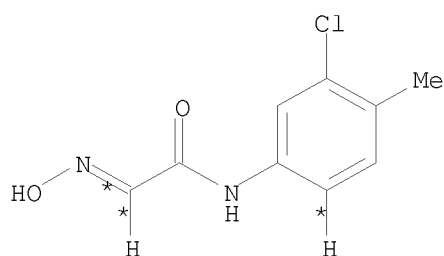
AU

START NEXT REACTION SEQUENCE

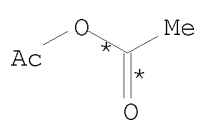
10/ 562,112



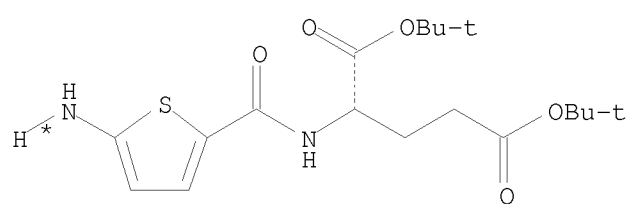
I



I

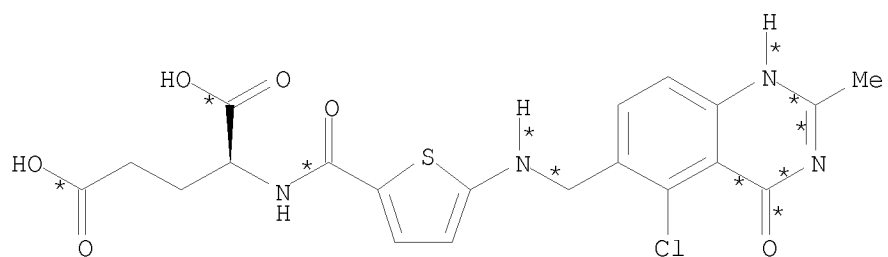


W



AU

7  
STEPS  
→



BF

YIELD 39%

RX(14) RCT B 6317-37-9

STAGE(1)

RGT AS 7719-09-7 SOC12

STAGE(2)

RCT AQ 16874-06-9

SOL 75-09-2 CH2Cl2

STAGE(3)

RGT AK 121-44-8 Et3N

PRO AR 450407-87-1

RX(15)

RCT AR 450407-87-1

RGT AV 7439-89-6 Fe

PRO AU 132463-36-6

10/ 562,112

CAT 7720-78-7 FeSO4  
SOL 67-56-1 MeOH

RX(3) RCT I 155184-79-5

STAGE(1)  
RGT N 7664-93-9 H2SO4

STAGE(2)  
SOL 67-64-1 Me2CO

PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2

STAGE(1)  
RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2  
SOL 7732-18-5 Water

STAGE(2)  
RGT S 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO P 155184-82-0

RX(8) RCT P 155184-82-0, W 108-24-7  
PRO X 450407-91-7  
SOL 108-24-7 Ac2O

RX(18) RCT X 450407-91-7

STAGE(1)  
RGT BB 7664-41-7 NH3

STAGE(2)  
RGT Q 1310-73-2 NaOH  
SOL 7732-18-5 Water

STAGE(3)  
RGT O 64-19-7 AcOH

PRO BC 450407-92-8

RX(19) RCT BC 450407-92-8  
RGT AN 128-08-5 Bromosuccinimide  
PRO BD 450407-93-9  
CAT 94-36-0 Benzoyl peroxide  
SOL 67-66-3 CHCl3

RX(20) RCT BD 450407-93-9, AU 132463-36-6  
RGT AZ 144-55-8 NaHCO3  
PRO BE 450407-94-0  
SOL 68-12-2 DMF

RX(21) RCT BE 450407-94-0

STAGE(1)  
RGT AD 76-05-1 F3CCO2H  
SOL 75-09-2 CH2Cl2

10/ 562,112

## STAGE (2)

RGT Q 1310-73-2 NaOH

SOL 7732-18-5 Water

### STAGE (3)

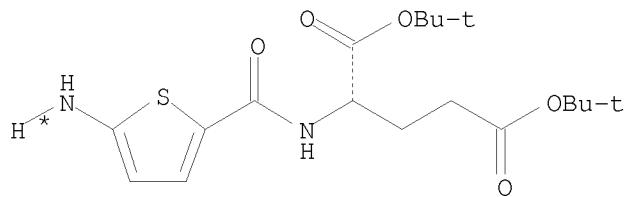
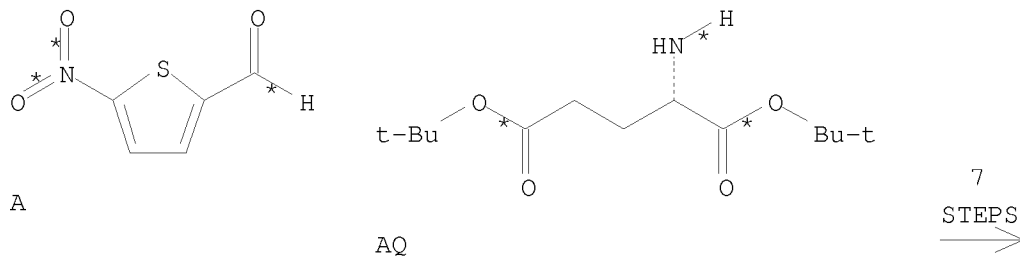
RGT 0 64-19-7 AcOH

PRO BF 450407-96-2

RX(189) OF 209 COMPOSED OF REACTION SEQUENCE RX(1), RX(14), RX(15), RX(20),  
RX(21)

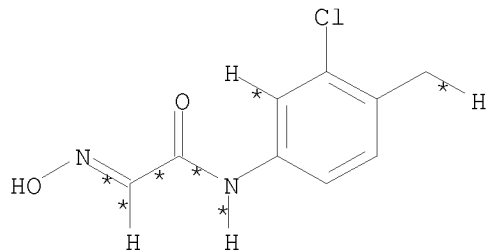
AND REACTION SEQUENCE RX(3), RX(6), RX(8), RX(18), RX(19),

RX(20), RX(21)

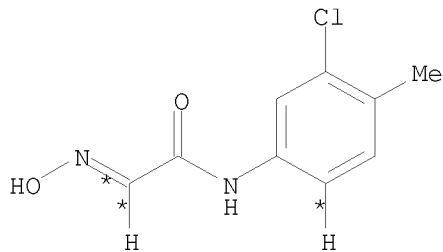
$$\dots A + AQ \implies AU \dots$$
$$\dots 2 \text{ I} + \text{W} + \text{AU} \implies \text{BF}$$


AU

START NEXT REACTION SEQUENCE

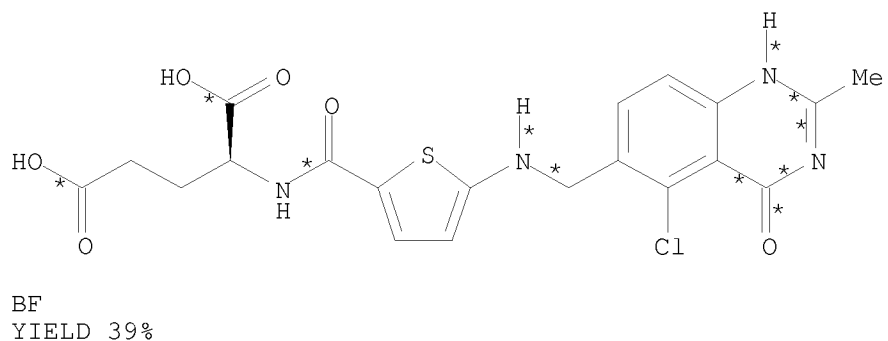
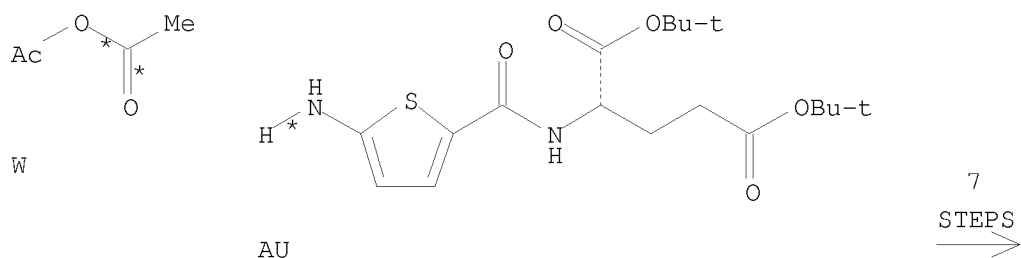


I



I

10/ 562,112



RX(1) RCT A 4521-33-9  
RGT C 7722-64-7 KMnO<sub>4</sub>, D 7558-80-7 NaH<sub>2</sub>PO<sub>4</sub>  
PRO B 6317-37-9  
SOL 7732-18-5 Water, 67-64-1 Me<sub>2</sub>CO

RX(14) RCT B 6317-37-9  
STAGE(1)  
RGT AS 7719-09-7 SOCl<sub>2</sub>

STAGE(2)  
RCT AQ 16874-06-9  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(3)  
RGT AK 121-44-8 Et<sub>3</sub>N

PRO AR 450407-87-1

RX(15) RCT AR 450407-87-1  
RGT AV 7439-89-6 Fe  
PRO AU 132463-36-6  
CAT 7720-78-7 FeSO<sub>4</sub>  
SOL 67-56-1 MeOH

RX(3) RCT I 155184-79-5  
STAGE(1)  
RGT N 7664-93-9 H<sub>2</sub>SO<sub>4</sub>  
STAGE(2)

SOL 67-64-1 Me2CO

PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2

STAGE(1)  
RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2  
SOL 7732-18-5 Water

STAGE(2)  
RGT S 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO P 155184-82-0

RX(8) RCT P 155184-82-0, W 108-24-7  
PRO X 450407-91-7  
SOL 108-24-7 Ac2O

RX(18) RCT X 450407-91-7

STAGE(1)  
RGT BB 7664-41-7 NH3

STAGE(2)  
RGT Q 1310-73-2 NaOH  
SOL 7732-18-5 Water

STAGE(3)  
RGT O 64-19-7 AcOH

PRO BC 450407-92-8

RX(19) RCT BC 450407-92-8  
RGT AN 128-08-5 Bromosuccinimide  
PRO BD 450407-93-9  
CAT 94-36-0 Benzoyl peroxide  
SOL 67-66-3 CHCl3

RX(20) RCT BD 450407-93-9, AU 132463-36-6  
RGT AZ 144-55-8 NaHCO3  
PRO BE 450407-94-0  
SOL 68-12-2 DMF

RX(21) RCT BE 450407-94-0

STAGE(1)  
RGT AD 76-05-1 F3CCO2H  
SOL 75-09-2 CH2Cl2

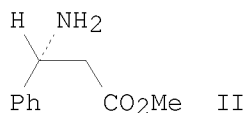
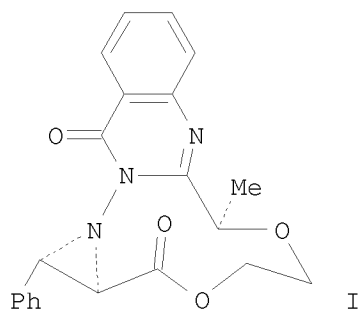
STAGE(2)  
RGT Q 1310-73-2 NaOH  
SOL 7732-18-5 Water

STAGE(3)  
RGT O 64-19-7 AcOH

PRO BF 450407-96-2

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 98 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 137:154915 CASREACT  
 TITLE: Completely diastereoselective aziridination of  $\alpha,\beta$ -unsaturated acids via intramolecular reaction of 3-acetoxyaminoquinazolin-4(3H)-ones  
 AUTHOR(S): Atkinson, Robert S.; Draycott, Richard D.; Hirst, David J.; Parratt, Martin J.; Raynham, Tony M.  
 CORPORATE SOURCE: Department of Chemistry, Leicester University, Leicester, LE1 7RH, UK  
 SOURCE: Tetrahedron Letters (2002), 43(11), 2083-2085  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

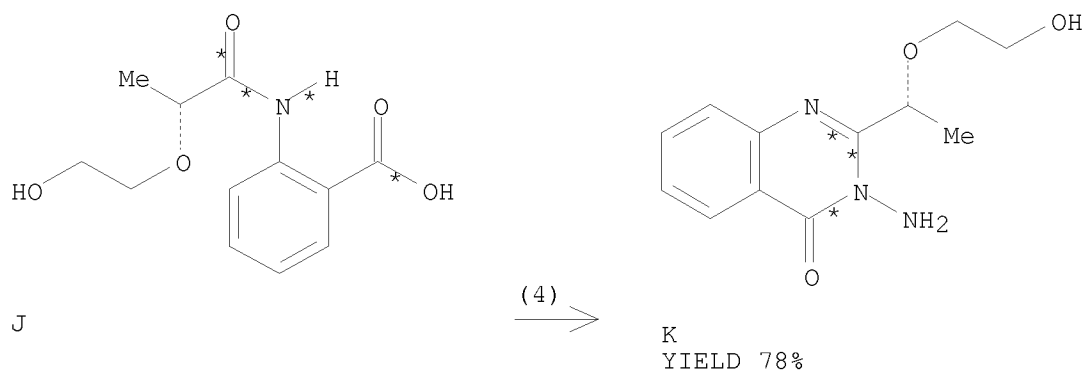


AB (R)-3-Amino-2-[1-(2-hydroxyethoxy)ethyl]quinazolin-4(3H)-one was prepared in 62% yield without the need for chromatog. and O-cinnamoylated; reaction with lead tetraacetate gave aziridine I as a single diastereoisomer in quant. yield which was converted into the  $\beta$ -amino acid ester II corresponding to overall enantioselective addition of ammonia to the double bond of cinnamic acid.

RX(4) OF 54 ...J ==> K...

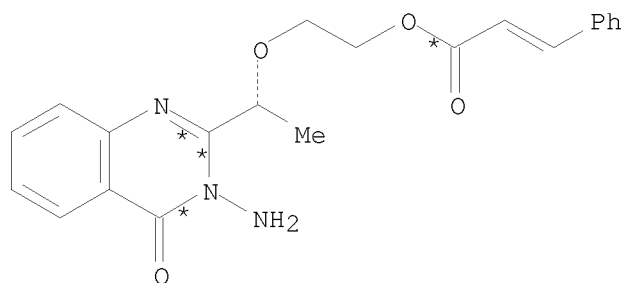
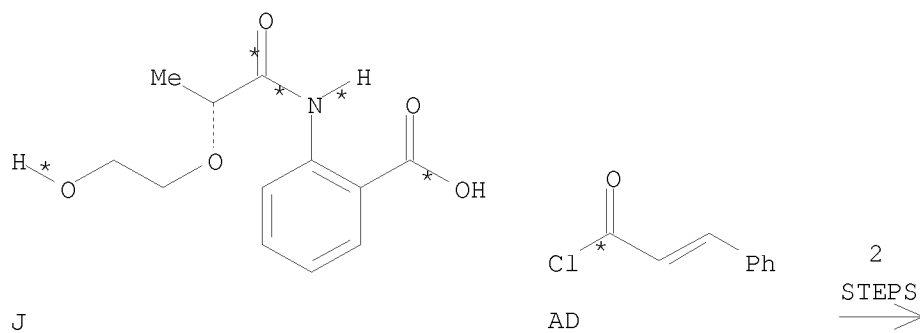


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RX(4) RCT J 445397-15-9  
RGT L 302-01-2 N2H4  
PRO K 445397-14-8  
SOL 64-17-5 EtOH

RX(16) OF 54 COMPOSED OF RX(4), RX(8)  
RX(16) J + AD ==> AE



AE  
YIELD 91%

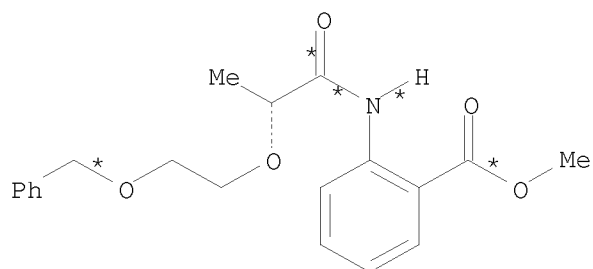
RX(4) RCT J 445397-15-9  
RGT L 302-01-2 N2H4

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PRO K 445397-14-8  
SOL 64-17-5 EtOH

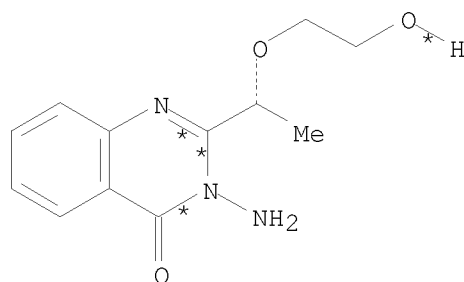
RX(8) RCT K 445397-14-8, AD 17082-09-6  
RGT Z 110-86-1 Pyridine  
PRO AE 445397-17-1  
SOL 75-09-2 CH2Cl2

RX(18) OF 54 COMPOSED OF RX(6), RX(4)  
RX(18) S ==> K



S

2  
STEPS  
→



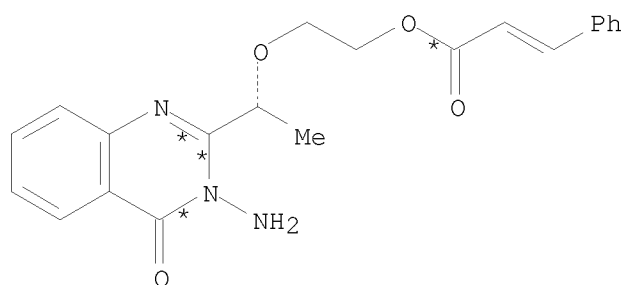
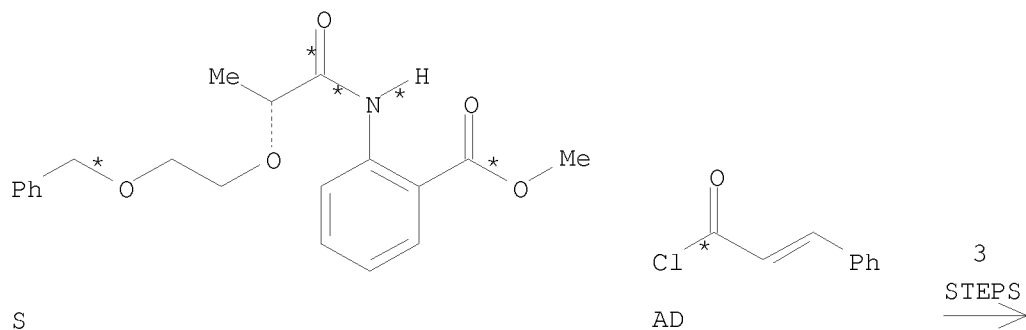
K  
YIELD 78%

RX(6) RCT S 445397-16-0  
RGT T 1333-74-0 H2  
PRO J 445397-15-9  
CAT 7440-05-3 Pd  
SOL 64-19-7 AcOH

RX(4) RCT J 445397-15-9  
RGT L 302-01-2 N2H4  
PRO K 445397-14-8  
SOL 64-17-5 EtOH

RX(30) OF 54 COMPOSED OF RX(6), RX(4), RX(8)  
RX(30) S + AD ==> AE

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AE  
YIELD 91%

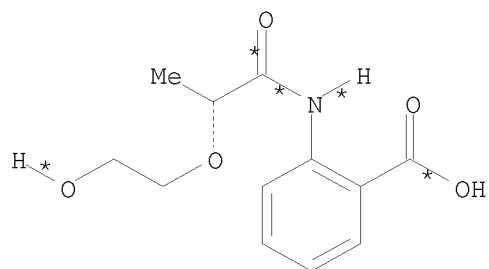
RX(6) RCT S 445397-16-0  
RGT T 1333-74-0 H2  
PRO J 445397-15-9  
CAT 7440-05-3 Pd  
SOL 64-19-7 AcOH

RX(4) RCT J 445397-15-9  
RGT L 302-01-2 N2H4  
PRO K 445397-14-8  
SOL 64-17-5 EtOH

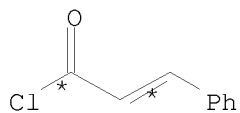
RX(8) RCT K 445397-14-8, AD 17082-09-6  
RGT Z 110-86-1 Pyridine  
PRO AE 445397-17-1  
SOL 75-09-2 CH2Cl2

RX(40) OF 54 COMPOSED OF RX(4), RX(8), RX(9), RX(10), RX(11)  
RX(40) J + AD + AA ==> AJ

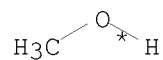
10/ 562,112



J

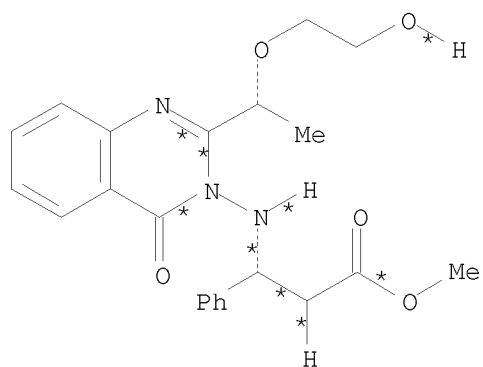


AD



AA

5  
STEPS  
→



AJ  
YIELD 95%

RX(4)      RCT    J 445397-15-9  
             RGT    L 302-01-2 N2H4  
             PRO    K 445397-14-8  
             SOL    64-17-5 EtOH

RX(8)      RCT    K 445397-14-8, AD 17082-09-6  
             RGT    Z 110-86-1 Pyridine  
             PRO    AE 445397-17-1  
             SOL    75-09-2 CH2Cl2

RX(9)      RCT    AE 445397-17-1  
             RGT    C 546-67-8 Pb(OAc)4, D 999-97-3 (Me3Si)2NH  
             PRO    AF 445397-18-2  
             SOL    75-09-2 CH2Cl2  
             NTE    stereoselective

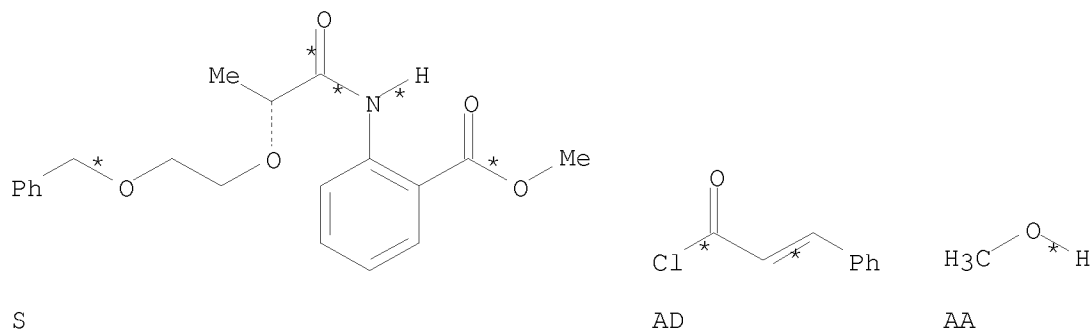
RX(10)     RCT    AF 445397-18-2  
             RGT    AH 32248-43-4 SmI2  
             PRO    AG 445397-19-3

10/ 562,112

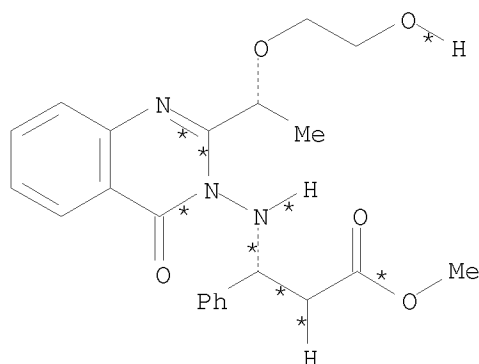
SOL 109-99-9 THF, 75-65-0 t-BuOH

RX(11) RCT AG 445397-19-3, AA 67-56-1  
RGT X 124-41-4 NaOMe  
PRO AJ 445397-20-6  
SOL 67-56-1 MeOH

RX(42) OF 54 COMPOSED OF RX(6), RX(4), RX(8), RX(9), RX(10), RX(11)  
RX(42) S + AD + AA ==> AJ



6  
STEPS  
→



AJ  
YIELD 95%

RX(6) RCT S 445397-16-0  
RGT T 1333-74-0 H2  
PRO J 445397-15-9  
CAT 7440-05-3 Pd  
SOL 64-19-7 AcOH

RX(4) RCT J 445397-15-9  
RGT L 302-01-2 N2H4  
PRO K 445397-14-8  
SOL 64-17-5 EtOH

RX(8) RCT K 445397-14-8, AD 17082-09-6  
RGT Z 110-86-1 Pyridine  
PRO AE 445397-17-1

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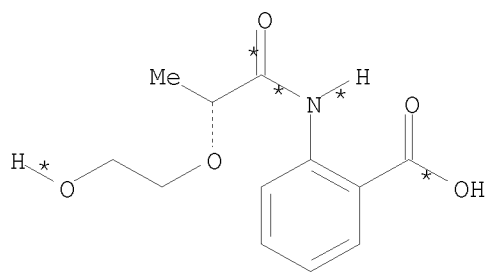
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(9) RCT AE 445397-17-1  
RGT C 546-67-8 Pb(OAc)<sub>4</sub>, D 999-97-3 (Me<sub>3</sub>Si)<sub>2</sub>NH  
PRO AF 445397-18-2  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
NTE stereoselective

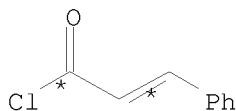
RX(10) RCT AF 445397-18-2  
RGT AH 32248-43-4 SmI<sub>2</sub>  
PRO AG 445397-19-3  
SOL 109-99-9 THF, 75-65-0 t-BuOH

RX(11) RCT AG 445397-19-3, AA 67-56-1  
RGT X 124-41-4 NaOMe  
PRO AJ 445397-20-6  
SOL 67-56-1 MeOH

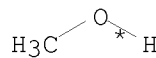
RX(51) OF 54 COMPOSED OF RX(4), RX(8), RX(9), RX(10), RX(11), RX(12)  
RX(51) J + AD + AA ==> AK + AL



J

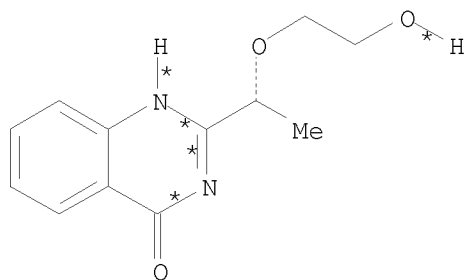


AD

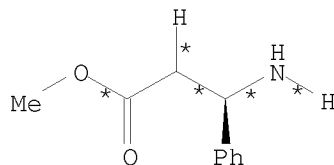


AA

6  
STEPS  
→



AK



AL

RX(4) RCT J 445397-15-9  
RGT L 302-01-2 N<sub>2</sub>H<sub>4</sub>

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PRO K 445397-14-8  
SOL 64-17-5 EtOH

RX(8) RCT K 445397-14-8, AD 17082-09-6  
RGT Z 110-86-1 Pyridine  
PRO AE 445397-17-1  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

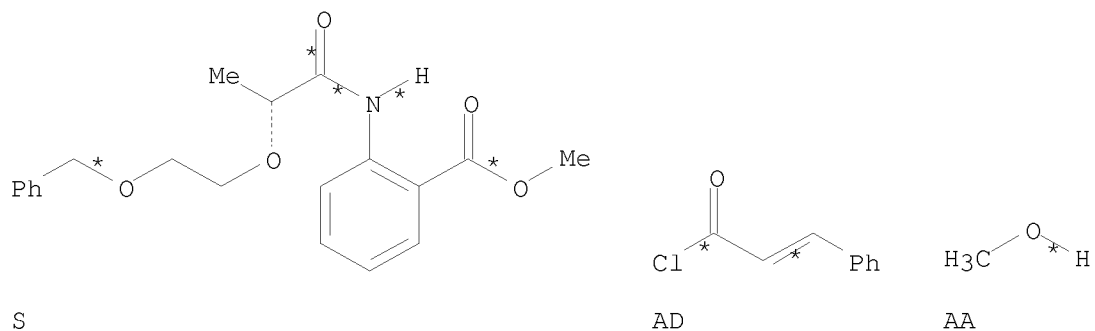
RX(9) RCT AE 445397-17-1  
RGT C 546-67-8 Pb(OAc)<sub>4</sub>, D 999-97-3 (Me<sub>3</sub>Si)<sub>2</sub>NH  
PRO AF 445397-18-2  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
NTE stereoselective

RX(10) RCT AF 445397-18-2  
RGT AH 32248-43-4 SmI<sub>2</sub>  
PRO AG 445397-19-3  
SOL 109-99-9 THF, 75-65-0 t-BuOH

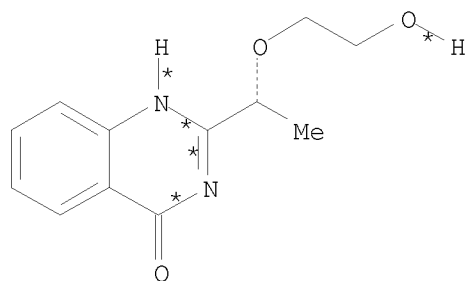
RX(11) RCT AG 445397-19-3, AA 67-56-1  
RGT X 124-41-4 NaOMe  
PRO AJ 445397-20-6  
SOL 67-56-1 MeOH

RX(12) RCT AJ 445397-20-6  
RGT AH 32248-43-4 SmI<sub>2</sub>, AM 108-01-0 Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>OH  
PRO AK 445397-21-7, AL 37088-67-8  
SOL 109-99-9 THF  
NTE 40% overall yield

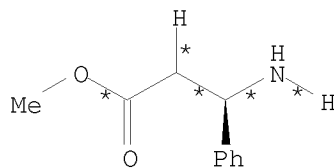
RX(52) OF 54 COMPOSED OF RX(6), RX(4), RX(8), RX(9), RX(10), RX(11), RX(12)  
RX(52) S + AD + AA ==> AK + AL



7  
STEPS  
→



AK



AL

RX(6)	RCT	S 445397-16-0
	RGT	T 1333-74-0 H2
	PRO	J 445397-15-9
	CAT	7440-05-3 Pd
	SOL	64-19-7 AcOH
RX(4)	RCT	J 445397-15-9
	RGT	L 302-01-2 N2H4
	PRO	K 445397-14-8
	SOL	64-17-5 EtOH
RX(8)	RCT	K 445397-14-8, AD 17082-09-6
	RGT	Z 110-86-1 Pyridine
	PRO	AE 445397-17-1
	SOL	75-09-2 CH2Cl2
RX(9)	RCT	AE 445397-17-1
	RGT	C 546-67-8 Pb(OAc)4, D 999-97-3 (Me3Si)2NH
	PRO	AF 445397-18-2
	SOL	75-09-2 CH2Cl2
	NTE	stereoselective
RX(10)	RCT	AF 445397-18-2
	RGT	AH 32248-43-4 SmI2
	PRO	AG 445397-19-3
	SOL	109-99-9 THF, 75-65-0 t-BuOH
RX(11)	RCT	AG 445397-19-3, AA 67-56-1
	RGT	X 124-41-4 NaOMe
	PRO	AJ 445397-20-6
	SOL	67-56-1 MeOH
RX(12)	RCT	AJ 445397-20-6
	RGT	AH 32248-43-4 SmI2, AM 108-01-0 Me2NCH2CH2OH
	PRO	AK 445397-21-7, AL 37088-67-8
	SOL	109-99-9 THF
	NTE	40% overall yield

REFERENCE COUNT:

16

THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



L3 ANSWER 99 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 137:47172 CASREACT

TITLE: Di-4(3H)-quinazolinon-2-yl derivatives from the diacid chlorides of pinic and sym-homopinic acids

AUTHOR(S): Avotin'sh, F. M.; Petrova, M. V.; Strakov, A. Ya.

CORPORATE SOURCE: Riga Technical University, Riga, LV-1658, Latvia

SOURCE: Chemistry of Heterocyclic Compounds (New York, NY, United States) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2001), 37(10), 1241-1243

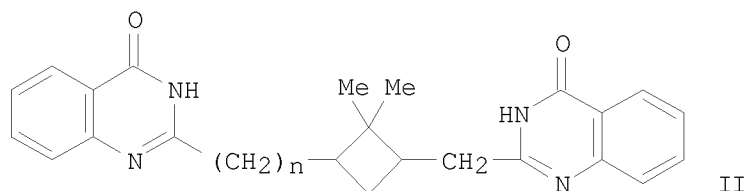
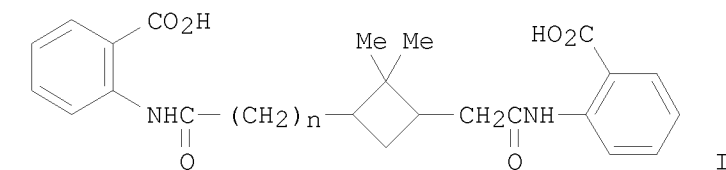
CODEN: CHCCAL; ISSN: 0009-3122

PUBLISHER: Kluwer Academic/Consultants Bureau

DOCUMENT TYPE: Journal

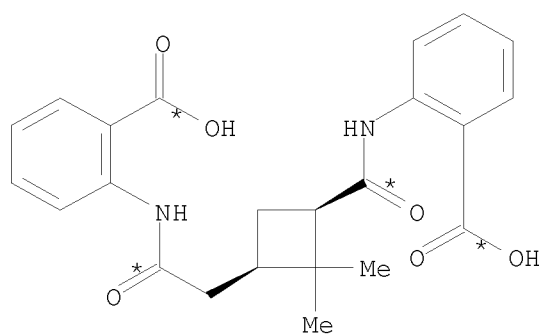
LANGUAGE: English

GI



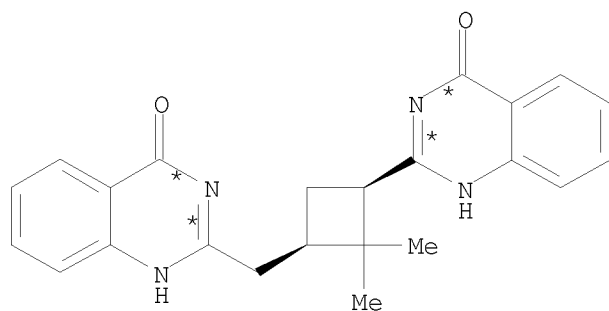
AB The corresponding dianthranilamides I ( $n = 0, 1$ ) were synthesized by the interaction of the diacid chlorides of *cis*-2,2-dimethyl-3-carboxycyclobutaneacetic acid (pinic acid) and *cis*-2,2-dimethylcyclobutane-1,3-diacetic acid (sym-homopinic acid) with two equivalent of anthranilic acid. Treatment of the dianthranilamides with formamide gave 2,2-dimethyl-1-[4(3H)-quinazolinon-2-yl]methyl-3-[4(3H)-quinazolinon-2-yl]cyclobutane II ( $n = 0$ ) and 2,2-dimethyl-1,3-di[4(3H)-quinazolinon-2-ylmethyl]cyclobutane II ( $n = 1$ ), resp.

RX(3) OF 8 ...C ==&gt; H



C

(3) →

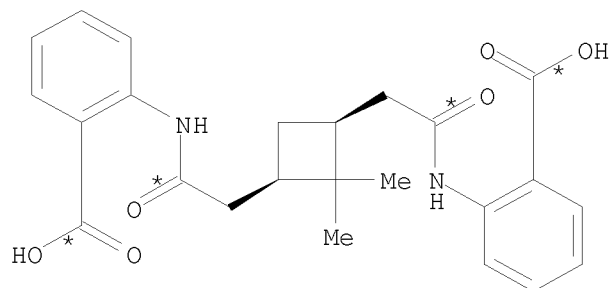


H

YIELD 69%

RX(3)      RCT    C 438001-74-2  
              PRO    H 438001-76-4  
              SOL    75-12-7 Formamide  
              NTE    thermal

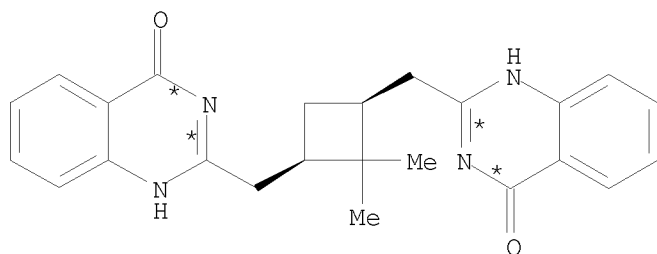
RX(4) OF 8      ...G ==&gt; J



G

(4) →

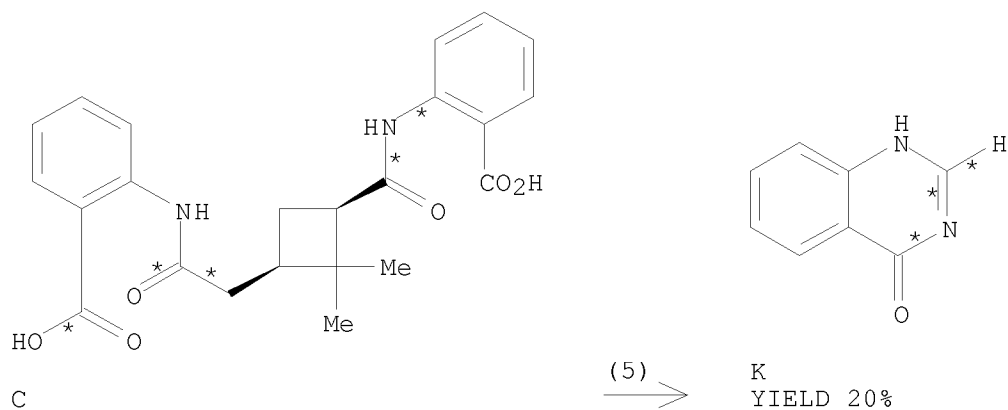
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J  
YIELD 65%

RX(4) RCT G 438001-75-3  
PRO J 438001-77-5  
SOL 75-12-7 Formamide  
NTE thermal

RX(5) OF 8 ...C ==> K

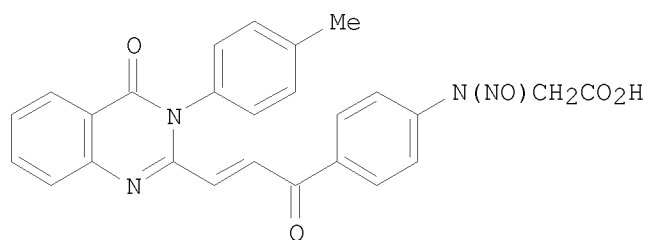


RX(5) RCT C 438001-74-2  
RGT L 7647-01-0 HCl  
PRO K 491-36-1  
SOL 7732-18-5 Water

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

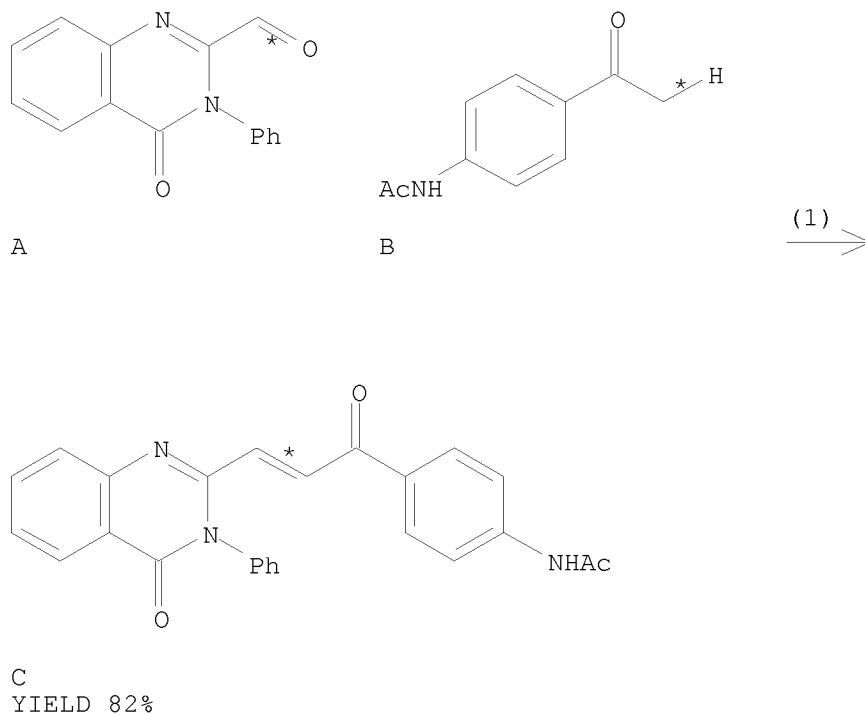
L3 ANSWER 100 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 136:294792 CASREACT  
TITLE: Synthesis and antimicrobial evaluation of chalcone and  
sydnone derivatives of 4(3H)-quinazolinone  
AUTHOR(S): Bekhit, Adnan A.; Habib, Nargues S.; Bekhit, El-Din A.  
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of  
Pharmacy, University of Alexandria, Alexandria, Egypt

SOURCE: Bollettino Chimico Farmaceutico (2001), 140(5), 297-301  
 CODEN: BCFAAI; ISSN: 0006-6648  
 PUBLISHER: Societa Editoriale Farmaceutica  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB The increasing clin. importance of drug-resistant bacterial pathogens has encouraged addnl. microbiol. and antibacterial research. New chalcone and sydnone derivs. of 4(3H)-quinazolinone were synthesized and evaluated for their antibacterial and antifungal activity. The microorganisms used were Escherichia coli ATCC 25922 as Gram-neg. bacteria, Staphylococcus aureus ATCC 19433 as Gram-Pos. bacteria and Candida albicans as yeast-like fungi. The most potent compound was the nitroso derivative I.

RX(1) OF 21      A + B ==> C



RX(1)      RCT    A 20873-11-4, B 2719-21-3

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STAGE(1)

RGT D 1310-73-2 NaOH

SOL 64-17-5 EtOH

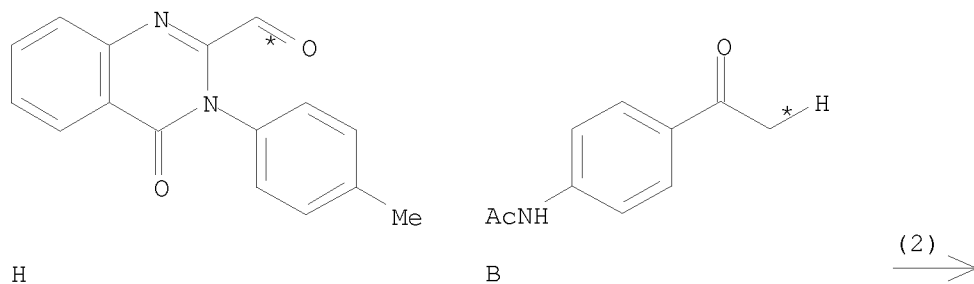
STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO C 407631-31-6

RX(2) OF 21 H + B ==> I



I  
YIELD 76%

RX(2) RCT H 53678-82-3, B 2719-21-3

STAGE(1)

RGT D 1310-73-2 NaOH

SOL 64-17-5 EtOH

STAGE(2)

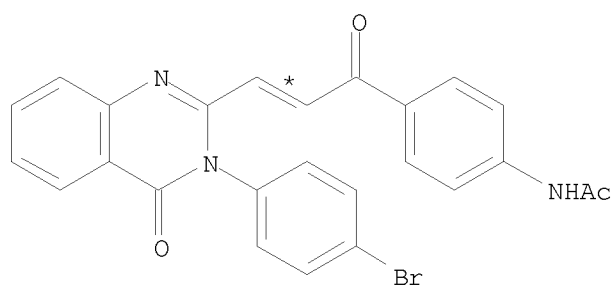
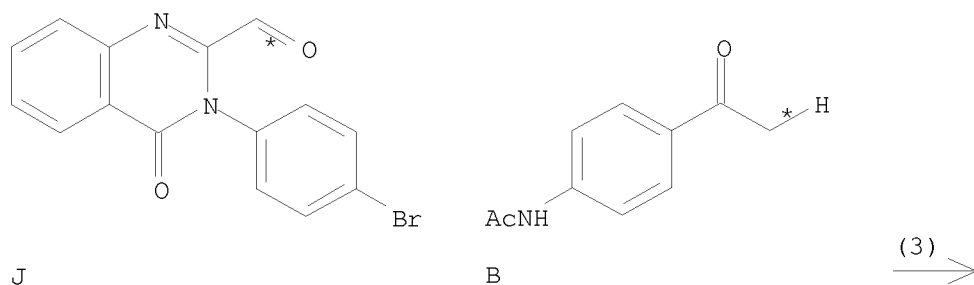
RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO I 407631-32-7

RX(3) OF 21 J + B ==> K

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K  
YIELD 87%

RX(3) RCT J 131532-68-8, B 2719-21-3

STAGE(1)

RGT D 1310-73-2 NaOH  
SOL 64-17-5 EtOH

STAGE(2)

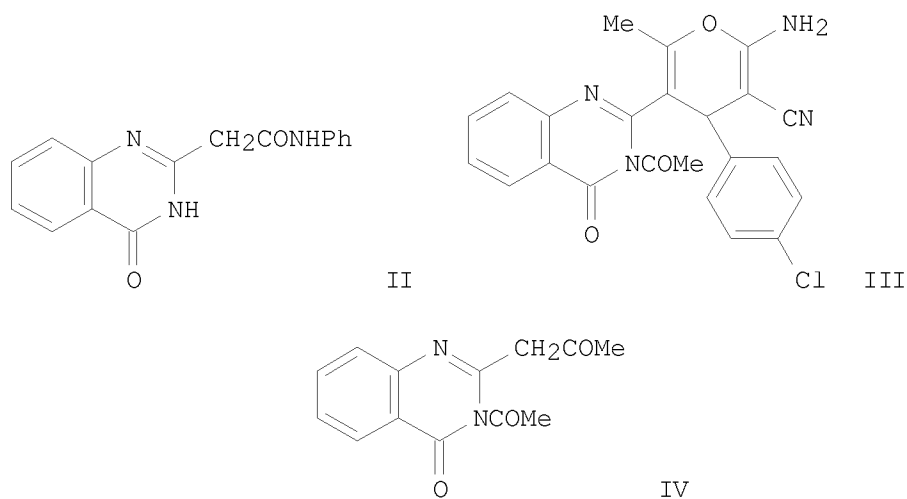
RGT E 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO K 407631-33-8

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

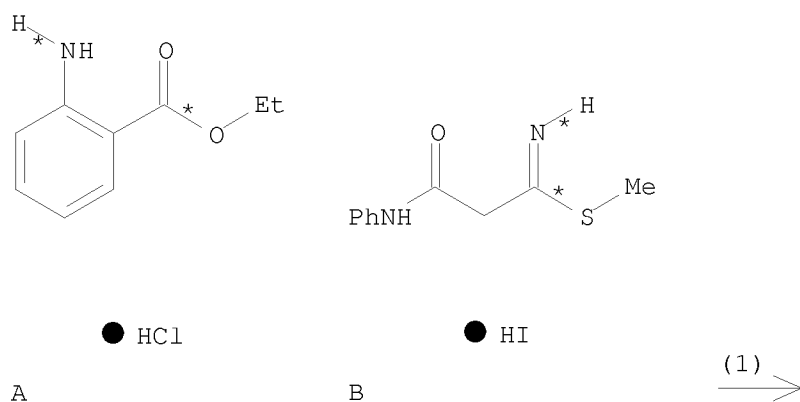
L3 ANSWER 101 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 136:247541 CASREACT  
TITLE: A new route for the synthesis of some quinazoline derivatives  
AUTHOR(S): Youssef, A. M. S.; Faty, Rasha A. M.  
CORPORATE SOURCE: Chemistry Department, Faculty of Science, Fayoum Branch, Cairo University, Fayoum, Egypt  
SOURCE: Egyptian Journal of Chemistry (2001), 44(4-6), 227-235  
CODEN: EGJCA3; ISSN: 0449-2285  
PUBLISHER: National Information and Documentation Centre  
DOCUMENT TYPE: Journal

LANGUAGE: English  
GI

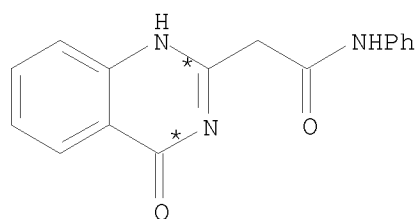


AB S-Me monothiomalonanilide hydroiodide (I) is a versatile compound for synthesizing quinazoline derivs. Thus, I reacted with either anthranilic acid or Et anthranilate hydrochloride to yield II. Also, polysubstituted pyranylquinazolinone III was obtained by reaction of quinazolinone derivative IV with p-chloro- $\alpha$ -cyanocinnamionitrile. Chemical and spectroscopic evidence for the structures of the newly synthesized compds. are described.

RX(1) OF 30 A + B ==> C...



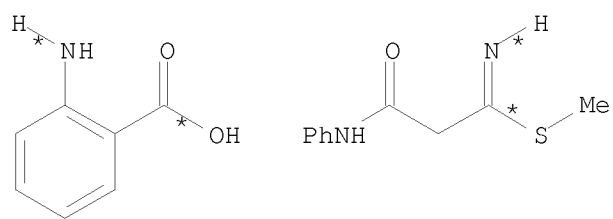
10/ 562,112



C  
YIELD 65%

RX(1)        RCT    A 32045-49-1, B 59750-09-3  
              RGT    D 127-09-3 AcONa  
              PRO    C 74089-31-9  
              SOL    64-17-5 EtOH

RX(2) OF 30        F   +   B   ==>   C...

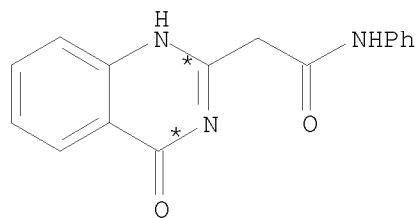


F

● HI

B

(2) >



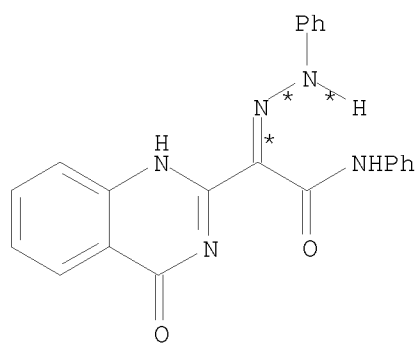
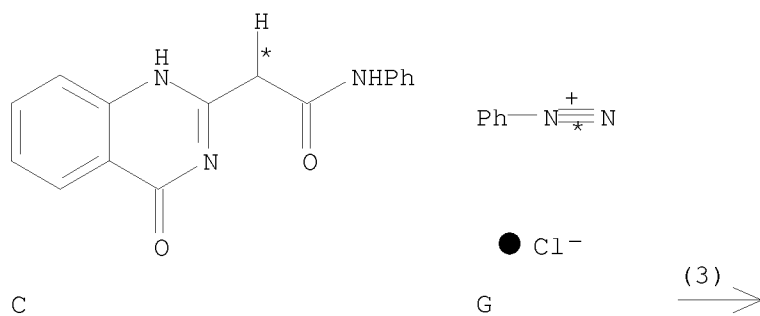
C

RX(2)        RCT    F 118-92-3, B 59750-09-3  
              PRO    C 74089-31-9  
              SOL    64-17-5 EtOH

RX(3) OF 30        ...C   +   G   ==>   H



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H  
YIELD 55%

RX(3)            RCT    C 74089-31-9

STAGE(1)

RGT    D 127-09-3 AcONa

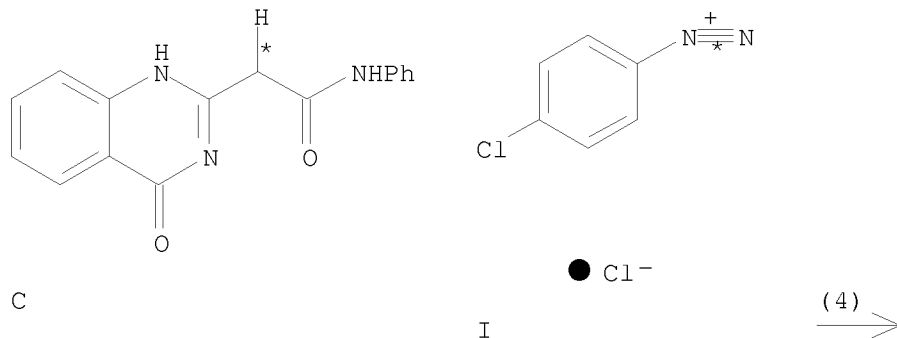
SOL    64-17-5 EtOH

STAGE(2)

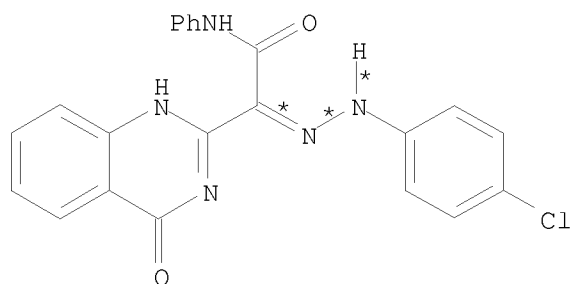
RCT    G 100-34-5

PRO    H 404384-07-2

RX(4) OF 30            ...C    +    I    ==>    J



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J  
YIELD 57%

RX(4) RCT C 74089-31-9

STAGE(1)

RGT D 127-09-3 AcONa

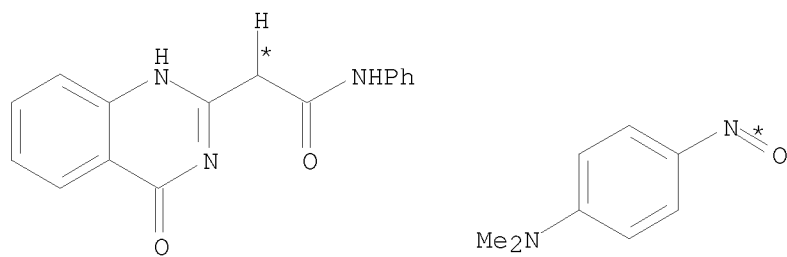
SOL 64-17-5 EtOH

STAGE(2)

RCT I 2028-74-2

PRO J 404384-08-3

RX(5) OF 30 ...C + K ==> L

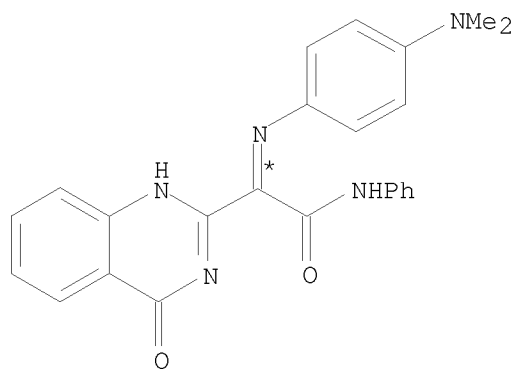


C

K

(5)  $\longrightarrow$

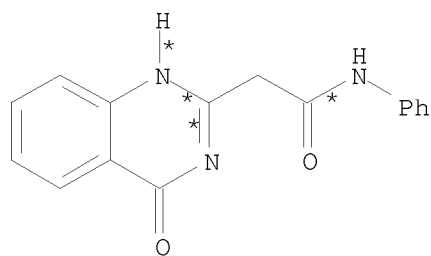
10/ 562,112



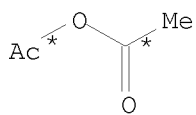
L  
YIELD 40%

RX(5)      RCT   C 74089-31-9, K 138-89-6  
              RGT   D 127-09-3 AcONa  
              PRO   L 404384-09-4  
              CAT   110-89-4 Piperidine  
              SOL   64-17-5 EtOH

RX(6) OF 30      ...C + N ==> O...

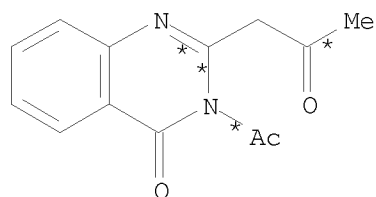


C



N

(6)  $\longrightarrow$



O  
YIELD 69%

RX(6)      RCT   C 74089-31-9, N 108-24-7

10/ 562,112

STAGE(1)

SOL 108-24-7 Ac2O

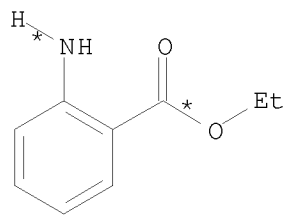
STAGE(2)

RGT P 7732-18-5 Water

PRO O 404384-10-7

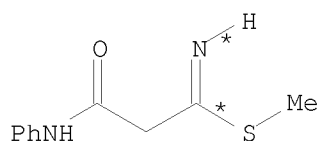
RX(11) OF 30 COMPOSED OF RX(1), RX(3)

RX(11) A + B + G ==> H



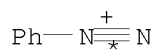
● HCl

A



● HI

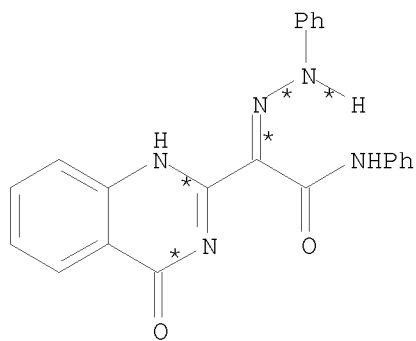
B



● Cl<sup>-</sup>

G

2  
STEPS  
→



H  
YIELD 55%

RX(1) RCT A 32045-49-1, B 59750-09-3  
RGT D 127-09-3 AcONa  
PRO C 74089-31-9  
SOL 64-17-5 EtOH

RX(3) RCT C 74089-31-9

STAGE(1)

RGT D 127-09-3 AcONa

SOL 64-17-5 EtOH

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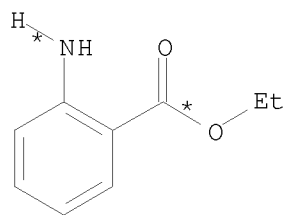
STAGE(2)

RCT G 100-34-5

PRO H 404384-07-2

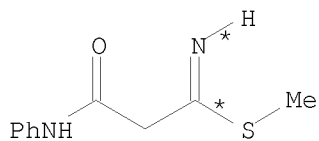
RX(12) OF 30 COMPOSED OF RX(1), RX(4)

RX(12) A + B + I ==> J



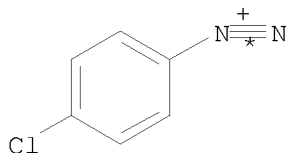
● HCl

A



● HI

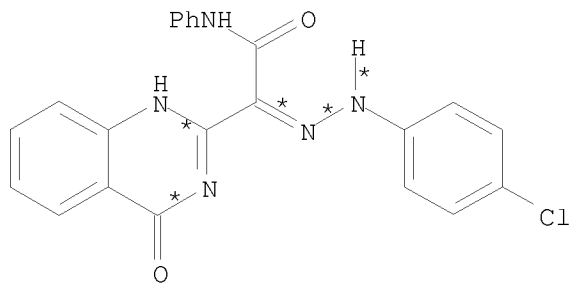
B



● Cl<sup>-</sup>

I

2  
STEPS  
→



J  
YIELD 57%

RX(1) RCT A 32045-49-1, B 59750-09-3  
RGT D 127-09-3 AcONa  
PRO C 74089-31-9  
SOL 64-17-5 EtOH

RX(4) RCT C 74089-31-9

STAGE(1)

RGT D 127-09-3 AcONa  
SOL 64-17-5 EtOH

STAGE(2)

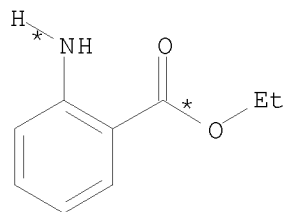
10/ 562,112

RCT I 2028-74-2

PRO J 404384-08-3

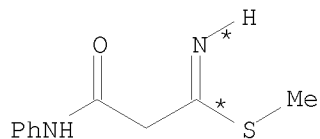
RX(13) OF 30 COMPOSED OF RX(1), RX(5)

RX(13) A + B + K ==> L



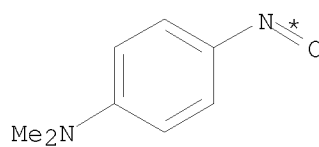
● HCl

A



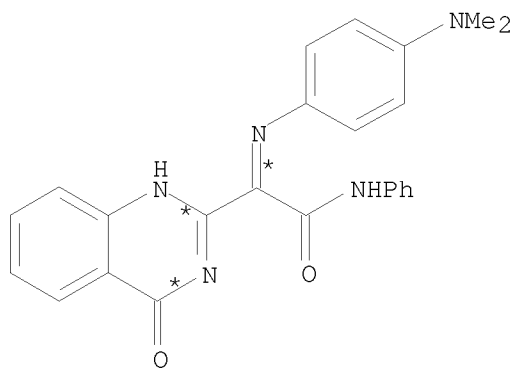
● HI

B



K

2  
STEPS  
→



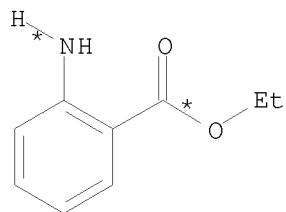
L  
YIELD 40%

RX(1) RCT A 32045-49-1, B 59750-09-3  
RGT D 127-09-3 AcONa  
PRO C 74089-31-9  
SOL 64-17-5 EtOH

RX(5) RCT C 74089-31-9, K 138-89-6  
RGT D 127-09-3 AcONa  
PRO L 404384-09-4  
CAT 110-89-4 Piperidine  
SOL 64-17-5 EtOH

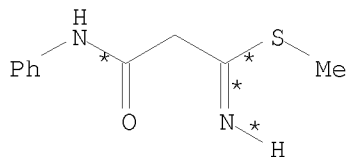
10/ 562,112

RX(14) OF 30 COMPOSED OF RX(1), RX(6)  
RX(14) A + B + N ==> O



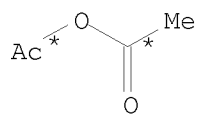
● HCl

A



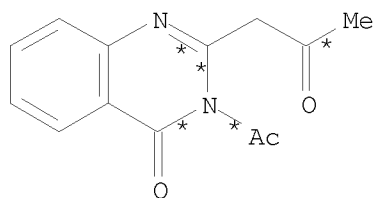
● HI

B



N

2  
STEPS  
=>



O  
YIELD 69%

RX(1) RCT A 32045-49-1, B 59750-09-3  
RGT D 127-09-3 AcONa  
PRO C 74089-31-9  
SOL 64-17-5 EtOH

RX(6) RCT C 74089-31-9, N 108-24-7

STAGE(1)  
SOL 108-24-7 Ac2O

STAGE(2)  
RGT P 7732-18-5 Water

PRO O 404384-10-7

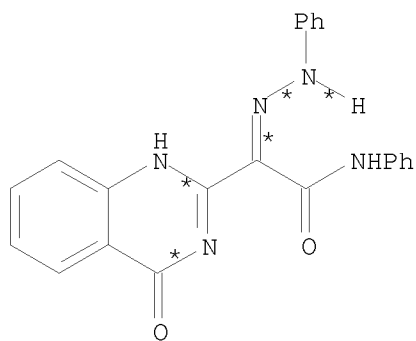
RX(15) OF 30 COMPOSED OF RX(2), RX(3)  
RX(15) F + B + G ==> H

O=C(O)c1ccccc1NCN(C)C(=O)CC(=O)Nc1ccccc1

● HI

● Cl<sup>-</sup>

2  
STEPS  
→



RX(2)            RCT    F 118-92-3, B 59750-09-3  
                  PRO    C 74089-31-9  
                  SOL    64-17-5 EtOH

STAGE (1)

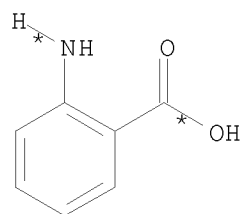
STAGE (2)

PRO H 404384-07-2

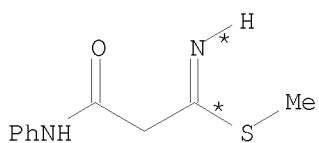
$$\text{RX (16)} \quad \text{F} + \text{B} + \text{I} \implies \text{J}$$



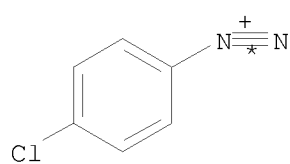
10/ 562,112



F

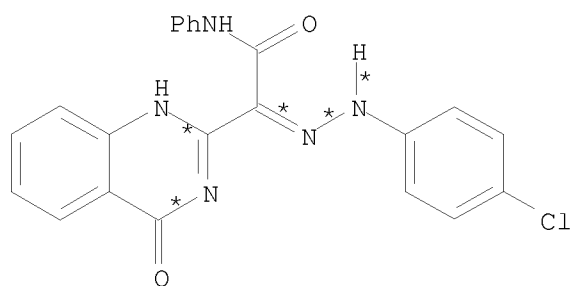


B



I

2  
STEPS  
→



J  
YIELD 57%

RX(2) RCT F 118-92-3, B 59750-09-3  
PRO C 74089-31-9  
SOL 64-17-5 EtOH

RX(4) RCT C 74089-31-9

STAGE(1)

RGT D 127-09-3 AcONa  
SOL 64-17-5 EtOH

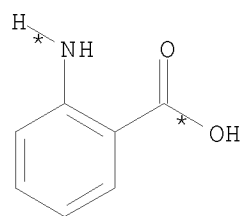
STAGE(2)

RCT I 2028-74-2

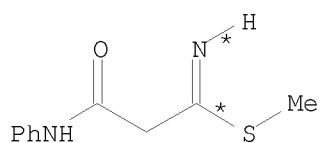
PRO J 404384-08-3

RX(17) OF 30 COMPOSED OF RX(2), RX(5)  
RX(17) F + B + K ==> L

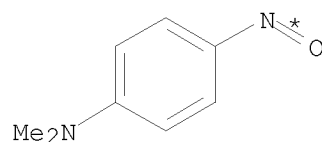
10/ 562,112



F

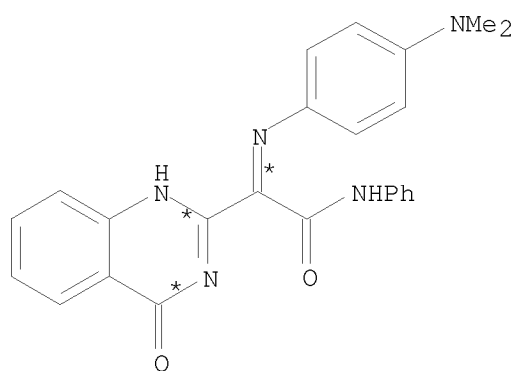


B



K

2  
STEPS  
→



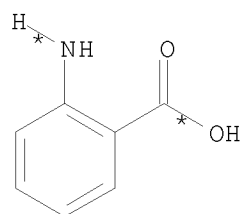
L

YIELD 40%

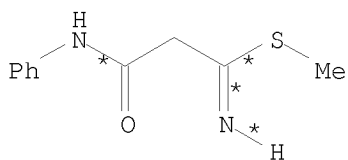
RX(2) RCT F 118-92-3, B 59750-09-3  
PRO C 74089-31-9  
SOL 64-17-5 EtOH

RX(5) RCT C 74089-31-9, K 138-89-6  
RGT D 127-09-3 AcONa  
PRO L 404384-09-4  
CAT 110-89-4 Piperidine  
SOL 64-17-5 EtOH

RX(18) OF 30 COMPOSED OF RX(2), RX(6)  
RX(18) F + B + N ==> O

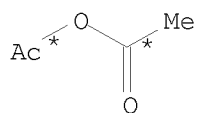


F



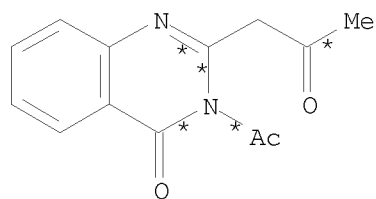
B

● HI



N

2  
STEPS  
→



O  
YIELD 69%

RX(2) RCT F 118-92-3, B 59750-09-3  
PRO C 74089-31-9  
SOL 64-17-5 EtOH

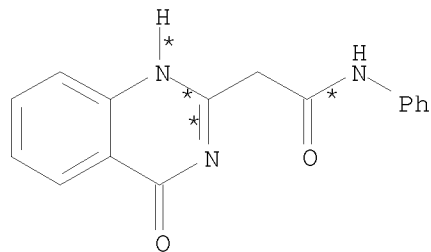
RX(6) RCT C 74089-31-9, N 108-24-7

STAGE(1)  
SOL 108-24-7 Ac2O

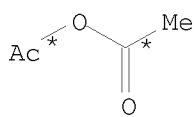
STAGE(2)  
RGT P 7732-18-5 Water

PRO O 404384-10-7

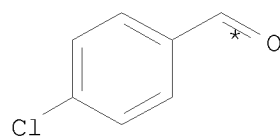
RX(19) OF 30 COMPOSED OF RX(6), RX(8)  
RX(19) C + N + T ==> U



C



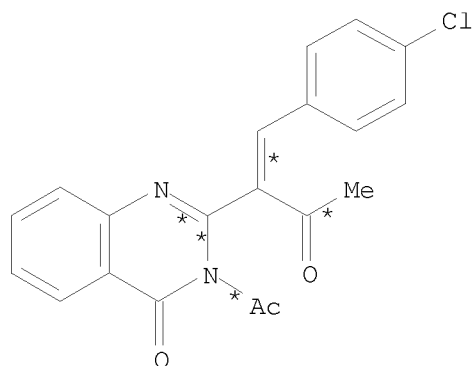
N



T

10/ 562,112

2  
STEPS  
→



U  
YIELD 35%

RX(6) RCT C 74089-31-9, N 108-24-7

STAGE(1)

SOL 108-24-7 Ac2O

STAGE(2)

RGT P 7732-18-5 Water

PRO O 404384-10-7

RX(8) RCT O 404384-10-7, T 104-88-1

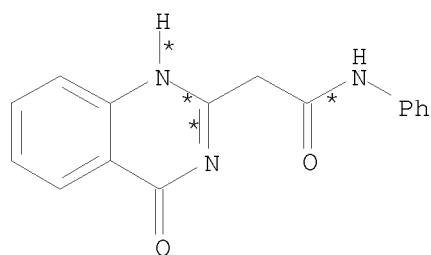
RGT D 127-09-3 AcONa

PRO U 404384-11-8

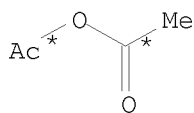
SOL 64-19-7 AcOH

RX(20) OF 30 COMPOSED OF RX(6), RX(9)

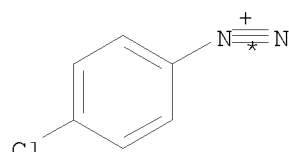
RX(20) C + N + I ==> W



C



N

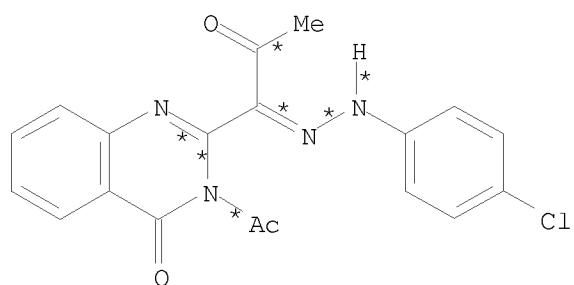


● Cl<sup>-</sup>

I

10/ 562,112

2  
STEPS  
→



W  
YIELD 63%

RX(6) RCT C 74089-31-9, N 108-24-7

STAGE(1)

SOL 108-24-7 Ac<sub>2</sub>O

STAGE(2)

RGT P 7732-18-5 Water

PRO O 404384-10-7

RX(9) RCT O 404384-10-7

STAGE(1)

RGT D 127-09-3 AcONa

SOL 64-17-5 EtOH

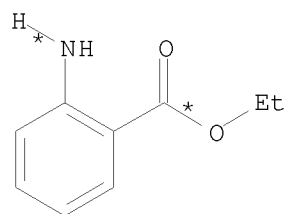
STAGE(2)

RCT I 2028-74-2

PRO W 404384-12-9

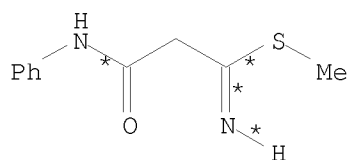
RX(25) OF 30 COMPOSED OF RX(1), RX(6), RX(8)

RX(25) A + B + N + T ==> U



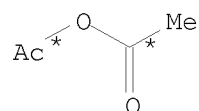
● HCl

A

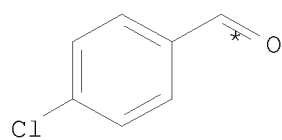


● HI

B

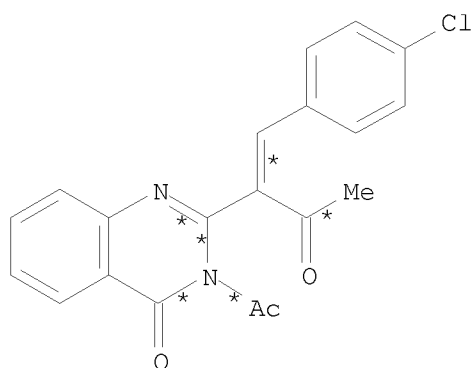


N



T

3  
STEPS  
→



U  
YIELD 35%

RX(1) RCT A 32045-49-1, B 59750-09-3  
RGT D 127-09-3 AcONa  
PRO C 74089-31-9  
SOL 64-17-5 EtOH

RX(6) RCT C 74089-31-9, N 108-24-7

STAGE(1)  
SOL 108-24-7 Ac2O

STAGE(2)  
RGT P 7732-18-5 Water

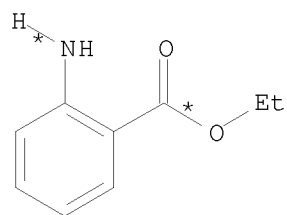
PRO O 404384-10-7

RX(8) RCT O 404384-10-7, T 104-88-1  
RGT D 127-09-3 AcONa  
PRO U 404384-11-8  
SOL 64-19-7 AcOH

RX(26) OF 30 COMPOSED OF RX(1), RX(6), RX(9)

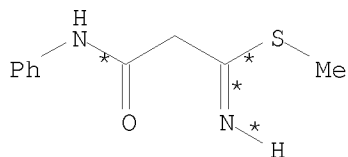
10/ 562,112

RX(26)      A + B + N + I ==> W



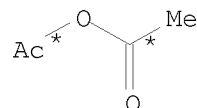
● HCl

A

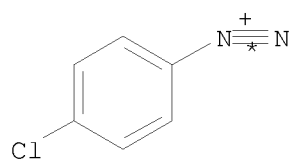


● HI

B



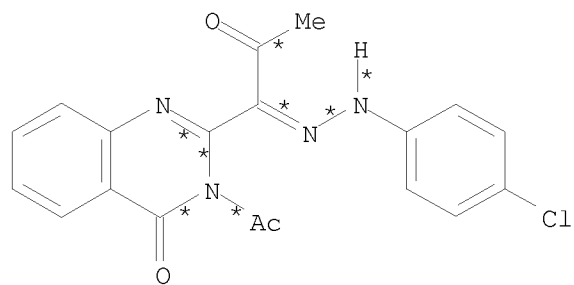
N



● Cl<sup>-</sup>

I

3  
STEPS  
→



W  
YIELD 63%

RX(1)      RCT    A 32045-49-1, B 59750-09-3  
              RGT    D 127-09-3 AcONa  
              PRO    C 74089-31-9  
              SOL    64-17-5 EtOH

RX(6)      RCT    C 74089-31-9, N 108-24-7

STAGE(1)

SOL    108-24-7 Ac2O

STAGE(2)

RGT    P 7732-18-5 Water

PRO    O 404384-10-7

RX(9)      RCT    O 404384-10-7

STAGE(1)

RGT    D 127-09-3 AcONa

SOL    64-17-5 EtOH

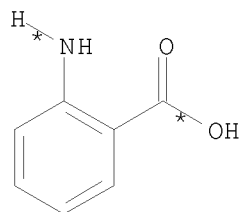
STAGE(2)

RCT    I 2028-74-2

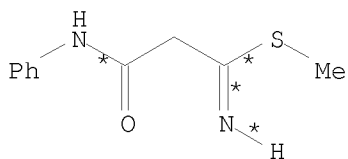
10/ 562,112

PRO W 404384-12-9

RX(28) OF 30 COMPOSED OF RX(2), RX(6), RX(8)  
RX(28) F + B + N + T ==> U

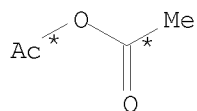


F

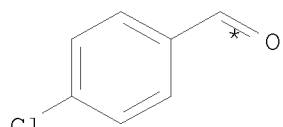


B

● HI

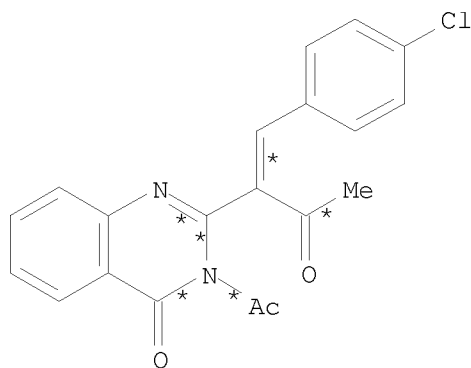


N



T

3  
STEPS  
→



U

YIELD 35%

RX(2) RCT F 118-92-3, B 59750-09-3  
PRO C 74089-31-9  
SOL 64-17-5 EtOH

RX(6) RCT C 74089-31-9, N 108-24-7

STAGE(1)

SOL 108-24-7 Ac2O



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STAGE(2)

RGT P 7732-18-5 Water

PRO O 404384-10-7

RX(8) RCT O 404384-10-7, T 104-88-1

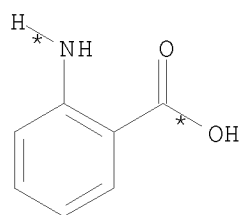
RGT D 127-09-3 AcONa

PRO U 404384-11-8

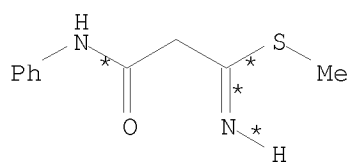
SOL 64-19-7 AcOH

RX(29) OF 30 COMPOSED OF RX(2), RX(6), RX(9)

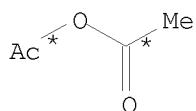
RX(29) F + B + N + I ==> W



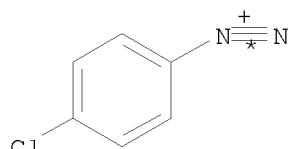
F



B



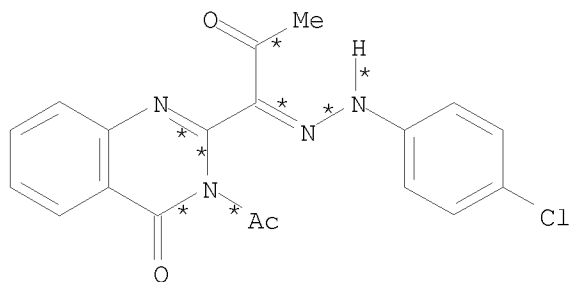
N



I



3  
STEPS  
→



W  
YIELD 63%

RX(2) RCT F 118-92-3, B 59750-09-3

PRO C 74089-31-9

SOL 64-17-5 EtOH

RX(6) RCT C 74089-31-9, N 108-24-7

STAGE(1)

SOL 108-24-7 Ac2O

STAGE(2)

RGT P 7732-18-5 Water

PRO O 404384-10-7

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RX(9) RCT O 404384-10-7

STAGE(1)

RGT D 127-09-3 AcONa

SOL 64-17-5 EtOH

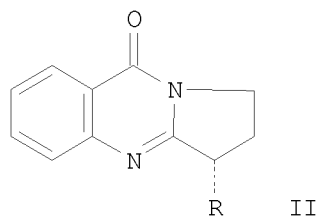
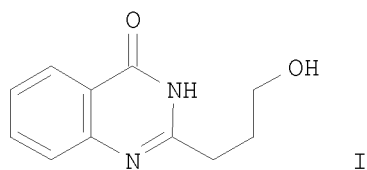
STAGE(2)

RCT I 2028-74-2

PRO W 404384-12-9

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 102 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 136:118618 CASREACT  
TITLE: Concise and Efficient Synthesis of Bioactive Natural Products Pegamine, Deoxyvasicinone, and (-)-Vasicinone  
AUTHOR(S): Mhaske, Santosh B.; Argade, Narshinha P.  
CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National Chemical Laboratory, Pune, 411 008, India  
SOURCE: Journal of Organic Chemistry (2001), 66(26), 9038-9040  
CODEN: JOCEAH; ISSN: 0022-3263  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

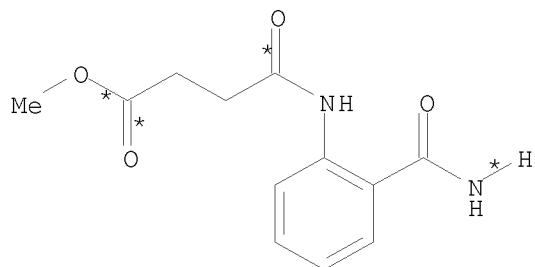


AB The authors have demonstrated a most concise, efficient, and practical synthesis of naturally occurring bioactive quinazolinone alkaloids pegamine (I), deoxyvasicinone (II, R = H), (-)-vasicinone (II, R = OH), for the first time starting from succinic anhydride and (S)-acetoxysuccinic anhydride. A formal synthesis of rutecarpine, isaindigotone, and luotonins A and B has been implied. The present approach also provides a new general method for designing several quinazolinone derivs. using a variety of cyclic anhydrides for structure

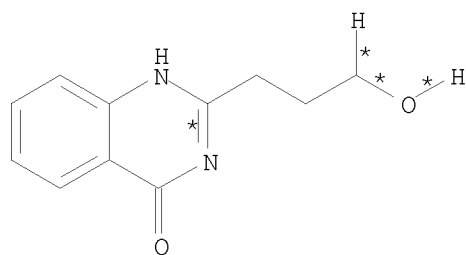
10/ 562,112

activity relationship studies.

RX(4) OF 32      ...M ==> A...



M



A

YIELD 93%

RX(4)      RCT    M 105234-41-1

STAGE(1)

RGT    O 16853-85-3 LiAlH<sub>4</sub>

SOL    109-99-9 THF

STAGE(2)

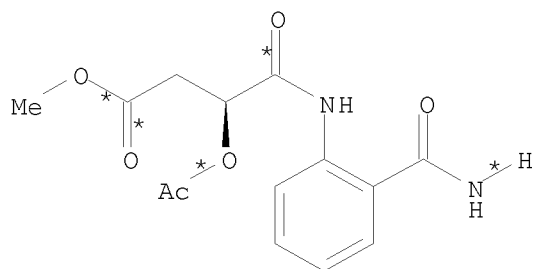
RGT    P 7732-18-5 Water

PRO    A 31431-93-3

NTE    chemoselective

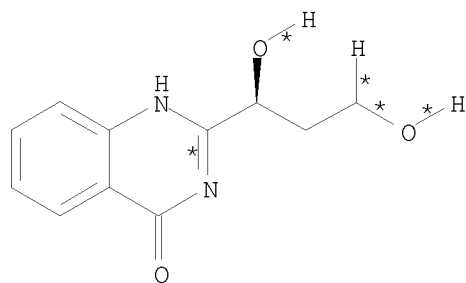
RX(8) OF 32      ...U ==> V...

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U

(8)  $\longrightarrow$



V

YIELD 92%

RX(8) RCT U 391249-54-0

STAGE(1)

RGT O 16853-85-3 LiAlH<sub>4</sub>

SOL 109-99-9 THF

STAGE(2)

RGT P 7732-18-5 Water

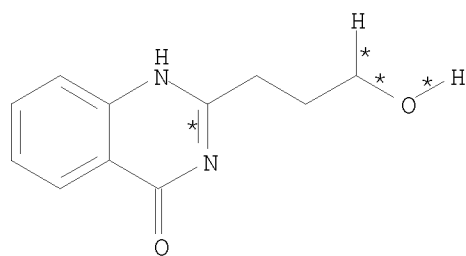
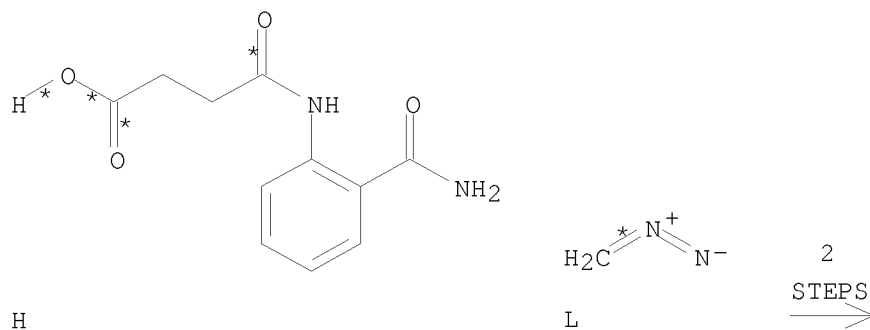
PRO V 391249-56-2

NTE stereoselective, chemoselective

RX(13) OF 32 COMPOSED OF RX(3), RX(4)

RX(13) H + L ==> A

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A  
YIELD 93%

RX(3) RCT H 306325-56-4, L 334-88-3

STAGE(1)  
SOL 60-29-7 Et<sub>2</sub>O

STAGE(2)  
RGT N 64-19-7 AcOH

PRO M 105234-41-1

RX(4) RCT M 105234-41-1

STAGE(1)  
RGT O 16853-85-3 LiAlH<sub>4</sub>  
SOL 109-99-9 THF

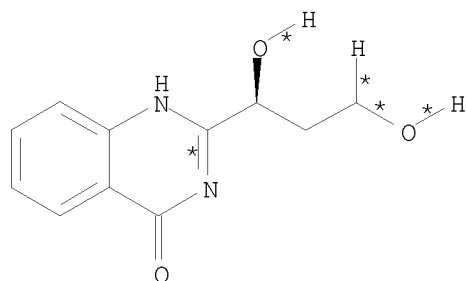
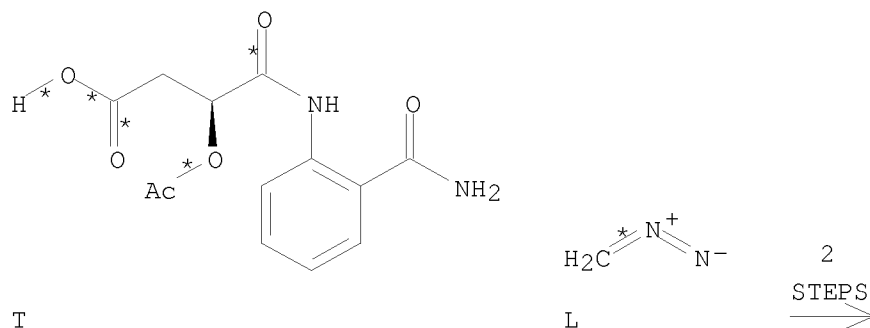
STAGE(2)  
RGT P 7732-18-5 Water

PRO A 31431-93-3  
NTE chemoselective

RX(17) OF 32 COMPOSED OF RX(7), RX(8)

RX(17) T + L ==> V

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YIELD 92%

RX(7) RCT T 391249-53-9, L 334-88-3

STAGE(1)

SOL 60-29-7 Et2O

STAGE(2)

RGT N 64-19-7 AcOH

PRO U 391249-54-0

NTE stereoselective

RX(8) RCT U 391249-54-0

STAGE(1)

RGT O 16853-85-3 LiAlH4

SOL 109-99-9 THF

STAGE(2)

RGT P 7732-18-5 Water

PRO V 391249-56-2

NTE stereoselective, chemoselective

REFERENCE COUNT:

64

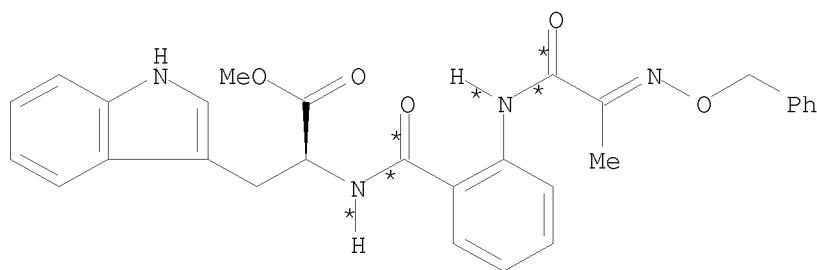
THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 103 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 135:152997 CASREACT  
TITLE: Synthesis of ent-Alantrypinone  
AUTHOR(S): Hart, David J.; Magomedov, Nabi A.  
CORPORATE SOURCE: Department of Chemistry, The Ohio State University,  
Columbus, OH, 43210, USA  
SOURCE: Journal of the American Chemical Society (2001),  
123(25), 5892-5899  
CODEN: JACSAT; ISSN: 0002-7863  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB This paper presents a synthesis of ent-alantrypinone, the enantiomer of a natural product produced by the fungus *Penicillium thymicola*. The synthesis revolves around the Li[Me<sub>3</sub>AlSPh]-promoted isomerization of iminobenzoxazine I to quinazolinone II, an N-acyliminium ion cyclization that converts enamide III to bridged indole, and rearrangement to oxindole title product. Ancillary chemical that involves thermal fragmentation of an iminobenzoxazine to a nitrile ylide and Me<sub>2</sub>AlSPh-mediated cyclization of oxime ether-ester to pyrrolidinone is also described.

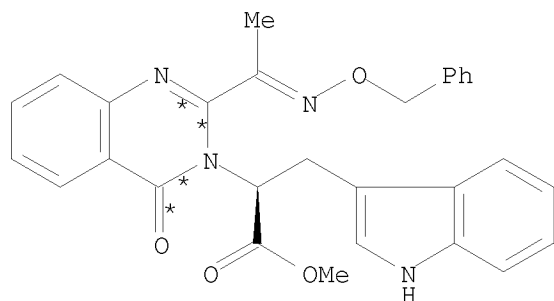
RX(39) OF 179 COMPOSED OF RX(11), RX(1)  
RX(39) AA ==> B



AA

2  
STEPS  
→

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B  
YIELD 90%

RX(11) RCT AA 352665-14-6  
RGT M 603-35-0 PPh3, AG 7553-56-2 I2, AH 7087-68-5 EtN(Pr-i)2  
PRO A 352665-17-9  
SOL 75-09-2 CH2Cl2

RX(1) RCT A 352665-17-9

STAGE(1)

RGT C 108-98-5 PhSH, D 109-72-8 BuLi  
SOL 75-09-2 CH2Cl2, 108-88-3 PhMe, 110-54-3 Hexane

STAGE(2)

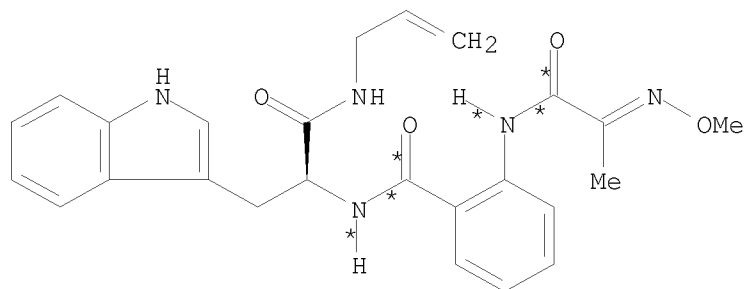
SOL 75-09-2 CH2Cl2

STAGE(3)

RGT E 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO B 352665-10-2

RX(42) OF 179 COMPOSED OF RX(16), RX(17)  
RX(42) AR ==> AU

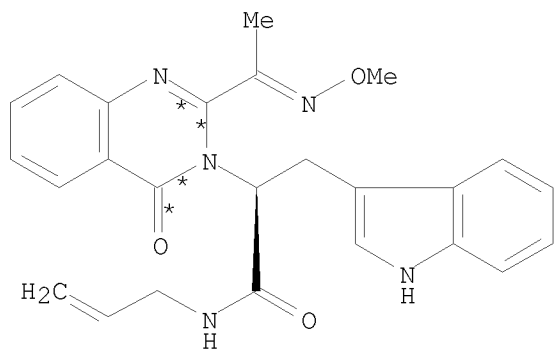


AR

2  
STEPS  
→



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AU

YIELD 93%

RX(16) RCT AR 352665-20-4  
RGT M 603-35-0 PPh3, AG 7553-56-2 I2, AH 7087-68-5 EtN(Pr-i)2  
PRO AS 352665-21-5  
SOL 75-09-2 CH2Cl2, 109-99-9 THF

RX(17) RCT AS 352665-21-5

STAGE (1)

RGT C 108-98-5 PhSH, D 109-72-8 BuLi

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 108-88-3 PhMe, 110-54-3 Hexane

STAGE (2)

SOL 75-09-2 CH2C12

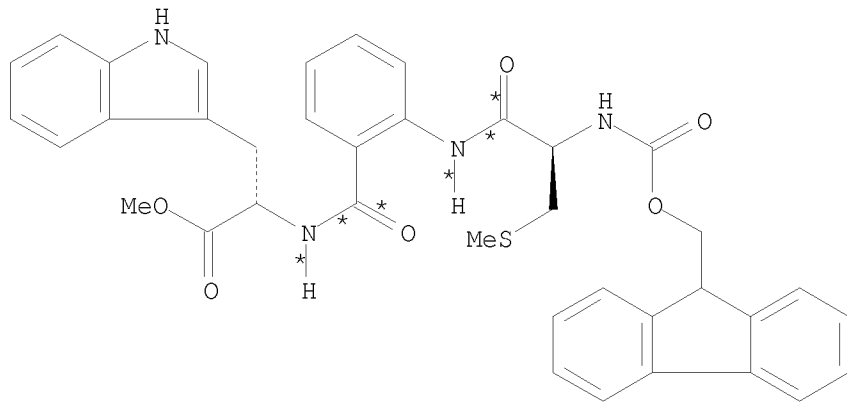
STAGE (3)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

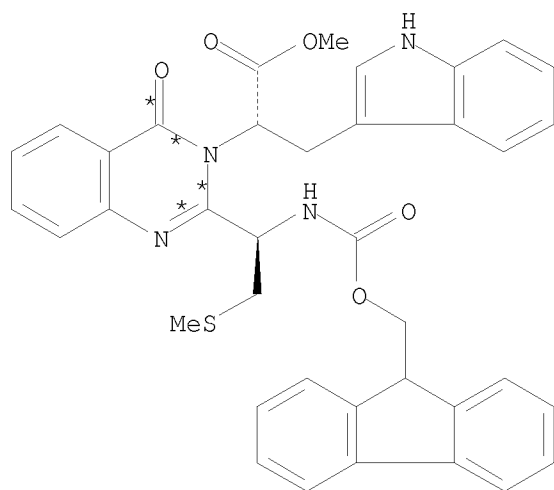
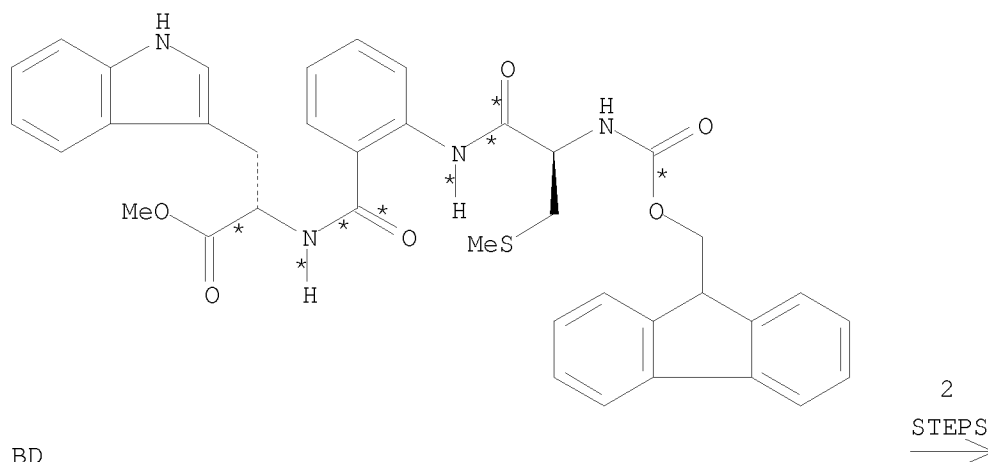
PRO AU 352665-22-6

RX(50) OF 179 COMPOSED OF RX(22), RX(23)

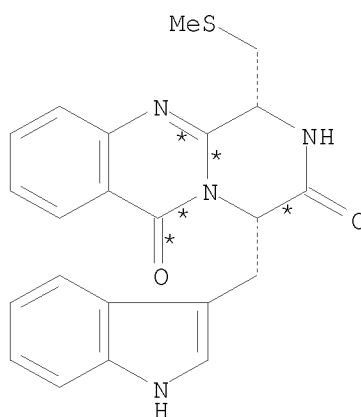
$$\text{RX (50)} \quad 2 \text{ BD} \implies \text{AV} + \text{J}$$


BD

10/ 562,112



YIELD 76%



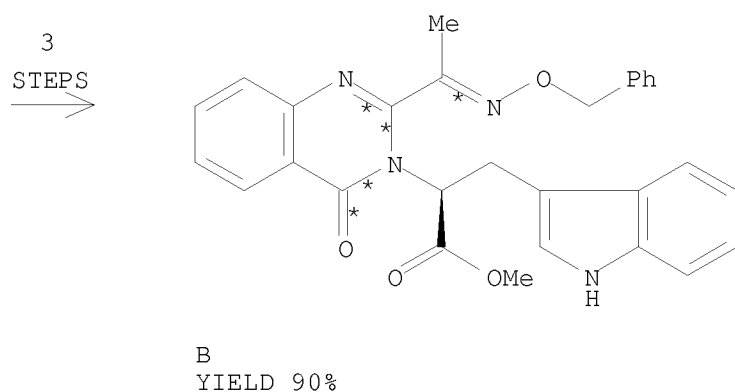
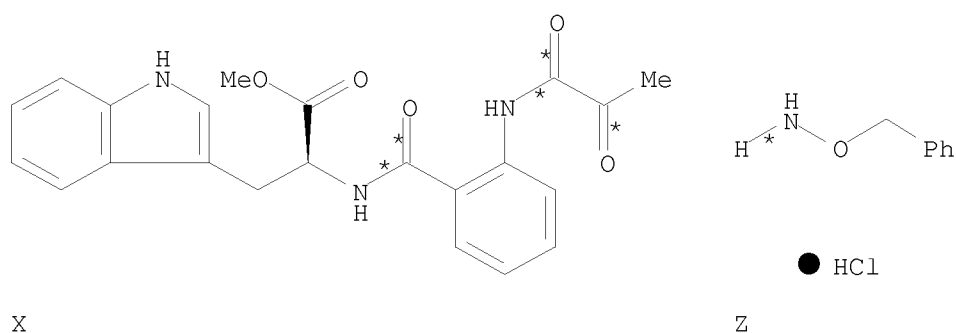
YIELD 8%

RX(22) RCT BD 246848-99-7  
RGT M 603-35-0 PPh3, AG 7553-56-2 I2, AH 7087-68-5 EtN(Pr-i)2  
PRO BF 246849-00-3  
SOL 75-09-2 CH2Cl2

RX(23) RCT BF 246849-00-3  
RGT C 108-98-5 PhSH, D 109-72-8 BuLi, V 75-24-1 AlMe3  
PRO AV 246849-02-5, J 246849-03-6  
SOL 109-99-9 THF, 110-54-3 Hexane, 108-88-3 PhMe

RX(72) OF 179 COMPOSED OF RX(7), RX(11), RX(1)  
RX(72) X + Z ==> B

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RX(7) RCT X 352665-12-4, Z 2687-43-6  
RGT AB 110-86-1 Pyridine  
PRO AA 352665-14-6  
SOL 67-56-1 MeOH

RX(11) RCT AA 352665-14-6  
RGT M 603-35-0 PPh3, AG 7553-56-2 I2, AH 7087-68-5 EtN(Pr-i)2  
PRO A 352665-17-9  
SOL 75-09-2 CH2Cl2

RX(1) RCT A 352665-17-9

STAGE(1)

RGT C 108-98-5 PhSH, D 109-72-8 BuLi  
SOL 75-09-2 CH2Cl2, 108-88-3 PhMe, 110-54-3 Hexane

STAGE(2)

SOL 75-09-2 CH2Cl2

STAGE(3)

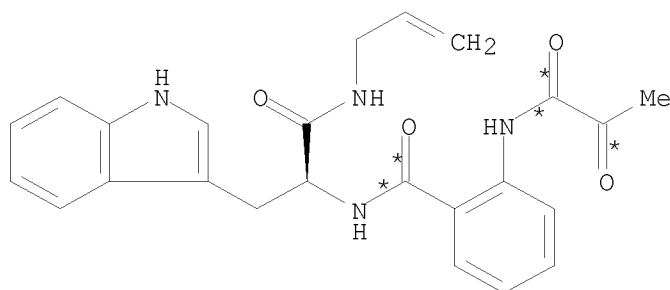
RGT E 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO B 352665-10-2

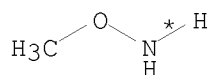
RX(74) OF 179 COMPOSED OF RX(15), RX(16), RX(17)

10/ 562,112

RX(74)      Y   +   AQ   ==>   AU



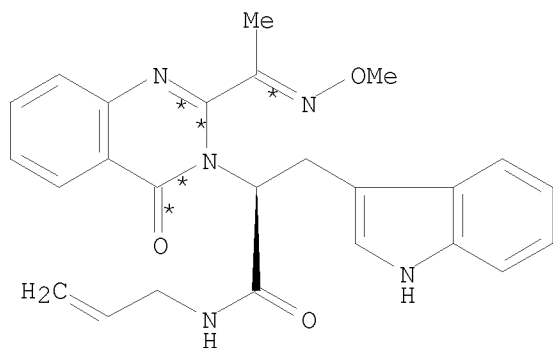
Y



● HCl

AQ

3  
STEPS  
→



AU  
YIELD 93%

RX(15)      RCT    Y 352665-13-5, AQ 593-56-6  
              RGT    AB 110-86-1 Pyridine  
              PRO    AR 352665-20-4  
              SOL    67-56-1 MeOH

RX(16)      RCT    AR 352665-20-4  
              RGT    M 603-35-0 PPh<sub>3</sub>, AG 7553-56-2 I<sub>2</sub>, AH 7087-68-5 EtN(Pr-i)<sub>2</sub>  
              PRO    AS 352665-21-5  
              SOL    75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 109-99-9 THF

RX(17)      RCT    AS 352665-21-5

STAGE(1)

              RGT    C 108-98-5 PhSH, D 109-72-8 BuLi  
              SOL    75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 108-88-3 PhMe, 110-54-3 Hexane

STAGE(2)

              SOL    75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

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STAGE(3)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO AU 352665-22-6

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 104 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 135:137461 CASREACT

TITLE: 2-[(3-Acetylamino-2,2-dimethylcyclobutyl)methyl]-4(3H)-quinazolinones

AUTHOR(S): Avotin'sh, F. M.; Petrova, M. V.; Tonkikh, N. N.; Strakov, A.

CORPORATE SOURCE: Riga Technical University, Riga, LV-1658, Latvia  
SOURCE: Chemistry of Heterocyclic Compounds (New York, NY, United States) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2000), 36(11), 1326-1328

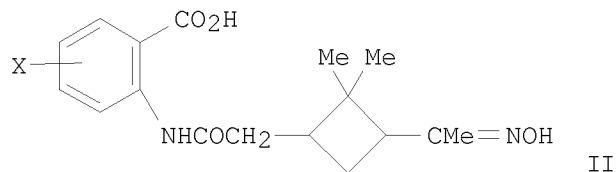
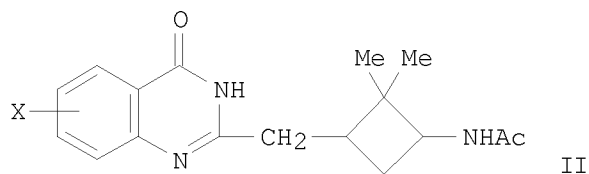
CODEN: CHCCAL; ISSN: 0009-3122

PUBLISHER: Consultants Bureau

DOCUMENT TYPE: Journal

LANGUAGE: English

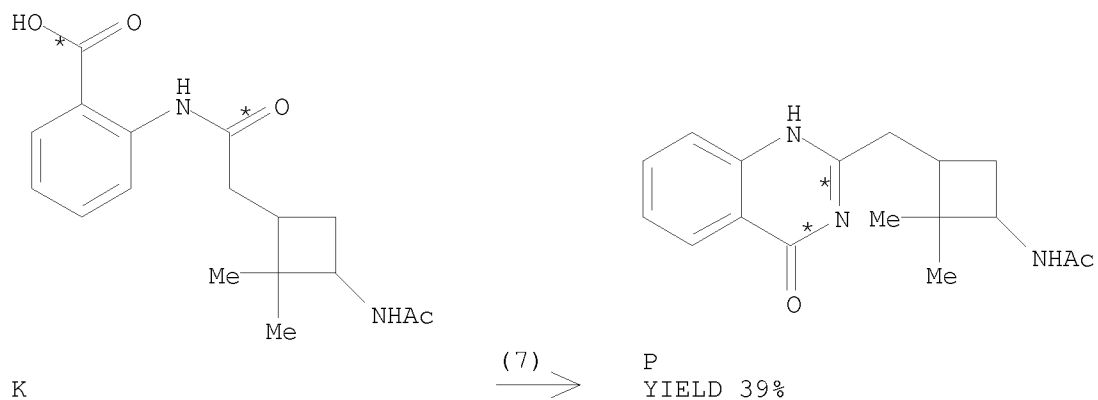
GI



AB The title compds. (I; X = H, 6-Br, 7-Cl) were prepared by Beckmann rearrangement of oximes II (X = 5-Br, 4-Cl), followed by cyclization with formamide.

RX(7) OF 18 ...K ==> P

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RX(7) RCT K 259262-89-0

STAGE(1)

RGT Q 75-12-7 Formamide

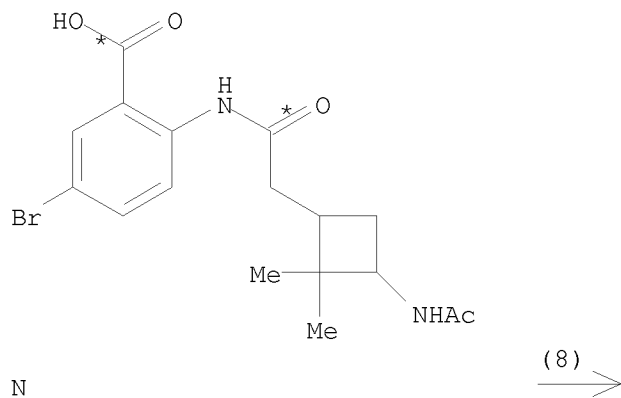
STAGE(2)

RGT R 144-55-8 NaHCO<sub>3</sub>

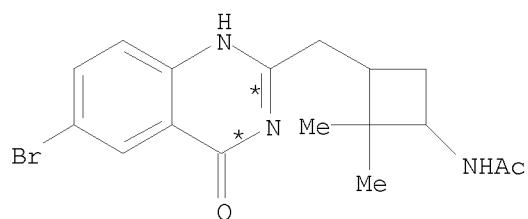
SOL 7732-18-5 Water

PRO P 352031-50-6

RX(8) OF 18 ...N ==> S



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S  
YIELD 41%

RX(8) RCT N 352031-48-2

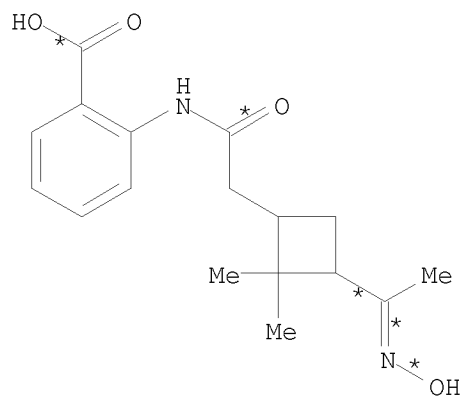
STAGE(1)  
RGT Q 75-12-7 Formamide

STAGE(2)  
RGT R 144-55-8 NaHCO3  
SOL 7732-18-5 Water

PRO S 352031-51-7

RX(13) OF 18 COMPOSED OF RX(4), RX(7)

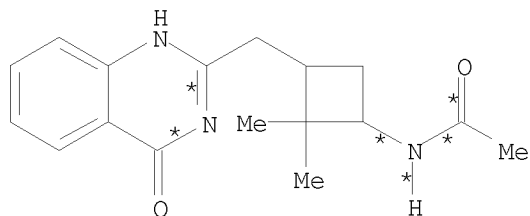
RX(13) B ==> P



B

2  
STEPS  
→

10/ 562,112



P  
YIELD 39%

RX(4) RCT B 259262-88-9

STAGE(1)

STAGE(2)

RGT L 1336-21-6 NH<sub>4</sub>OH

SOL 7732-18-5 Water

STAGE(3)

SOL 141-78-6 AcOEt

PRO K 259262-89-0

NTE polyphosphoric acid used in first stage

RX(7) RCT K 259262-89-0

STAGE(1)

RGT Q 75-12-7 Formamide

STAGE(2)

RGT R 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water

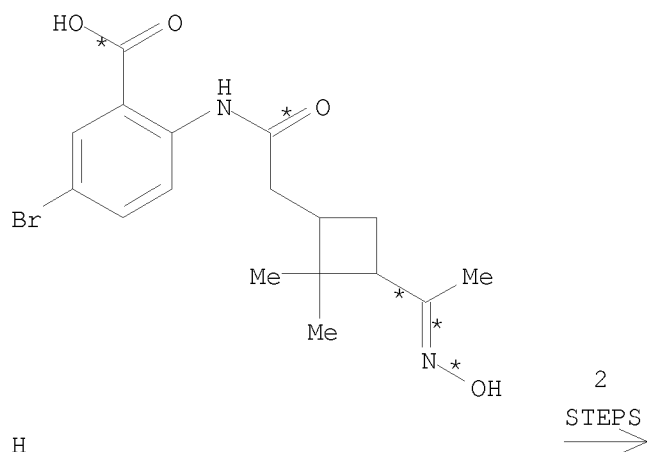
PRO P 352031-50-6

RX(14) OF 18 COMPOSED OF RX(5), RX(8)

RX(14) H ==> S



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S  
YIELD 41%

RX(5) RCT H 352031-46-0

STAGE(1)

STAGE(2)

RGT L 1336-21-6 NH4OH

SOL 7732-18-5 Water

STAGE(3)

SOL 141-78-6 AcOEt

PRO N 352031-48-2

RX(8) RCT N 352031-48-2

STAGE(1)

RGT Q 75-12-7 Formamide

STAGE(2)

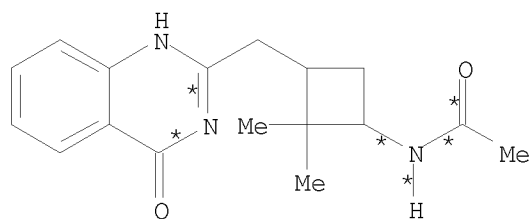
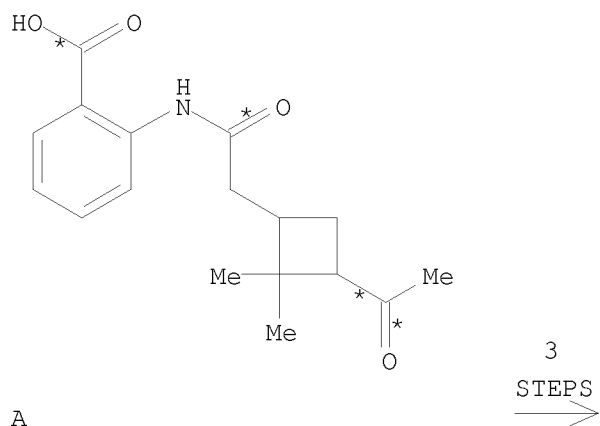
RGT R 144-55-8 NaHCO3

SOL 7732-18-5 Water

PRO S 352031-51-7

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RX(16) OF 18 COMPOSED OF RX(1), RX(4), RX(7)  
RX(16) A ==> P



YIELD 39%

RX(1) RCT A 259262-85-6

STAGE(1)

RGT C 5470-11-1 H2NOH-HCl, D 127-09-3 AcONa  
SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO B 259262-88-9

RX(4) RCT B 259262-88-9

STAGE(1)

STAGE(2)

RGT L 1336-21-6 NH4OH  
SOL 7732-18-5 Water

STAGE(3)

SOL 141-78-6 AcOEt

PRO K 259262-89-0

NTE polyphosphoric acid used in first stage

10/ 562,112

RX(7) RCT K 259262-89-0

STAGE(1)

RGT Q 75-12-7 Formamide

STAGE(2)

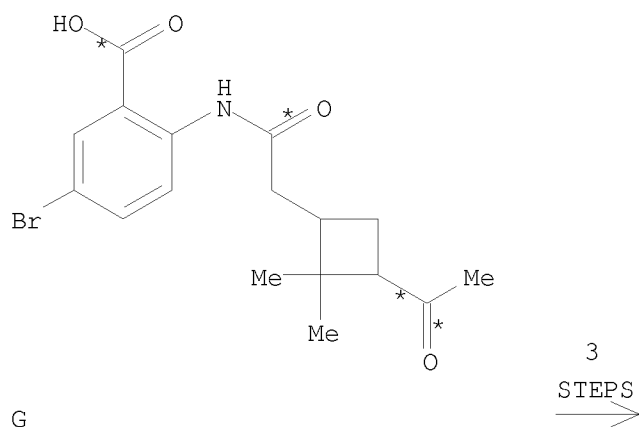
RGT R 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water

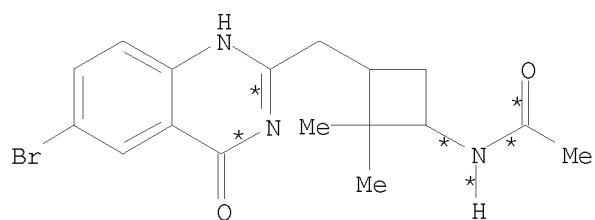
PRO P 352031-50-6

RX(17) OF 18 COMPOSED OF RX(2), RX(5), RX(8)

RX(17) G ==> S



G



S

YIELD 41%

RX(2) RCT G 259262-86-7

STAGE(1)

RGT C 5470-11-1 H<sub>2</sub>NOH-HCl, D 127-09-3 AcONa

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO H 352031-46-0

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RX(5) RCT H 352031-46-0

STAGE(1)

STAGE(2)

RGT L 1336-21-6 NH4OH  
SOL 7732-18-5 Water

STAGE(3)

SOL 141-78-6 AcOEt

PRO N 352031-48-2

RX(8) RCT N 352031-48-2

STAGE(1)

RGT Q 75-12-7 Formamide

STAGE(2)

RGT R 144-55-8 NaHCO3  
SOL 7732-18-5 Water

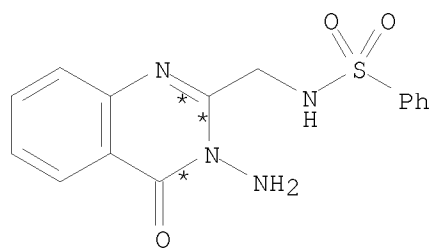
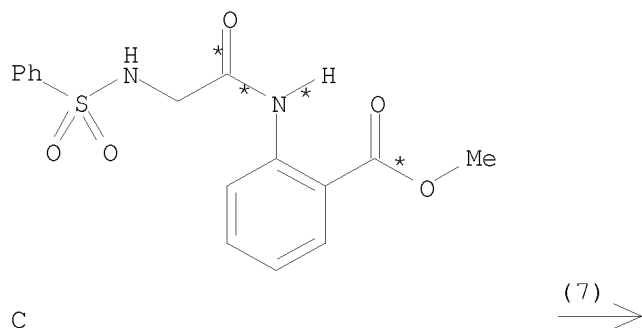
PRO S 352031-51-7

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 105 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 135:122713 CASREACT  
TITLE: Amino acids in the synthesis of heterocyclic systems:  
The synthesis of triazinoquinazolinones,  
triazepinoquinazolinones and triazocinoquinazolinones  
of potential biological interest  
AUTHOR(S): El-Sharief, A. M. Sh.; Ammar, Y. A.; Zahran, M. A.;  
Ali, A. H.; El-Gaby, M. S. A.  
CORPORATE SOURCE: Dep. Chemistry, Faculty Science, Al-Azhar Univ.,  
Nasr-City, 11884, Egypt  
SOURCE: Molecules [online computer file] (2001), 6(3), 267-278  
CODEN: MOLEFW; ISSN: 1420-3049  
URL: <http://www.mdpi.org/molecules/papers/60300267.pdf>  
PUBLISHER: Molecular Diversity Preservation International  
DOCUMENT TYPE: Journal; (online computer file)  
LANGUAGE: English  
AB A number of novel triazino-, triazepino- and triazocinoquinazolinones were  
obtained by nucleophilic reactions of 3-aminoquinazolinone derivs.  
obtained by condensation of arylsulfonyl amino acids with Me anthranilate,  
followed by hydrazinolysis. Some of the products showed antimicrobial and  
antifungal activities.

RX(7) OF 76 ...C ==> P

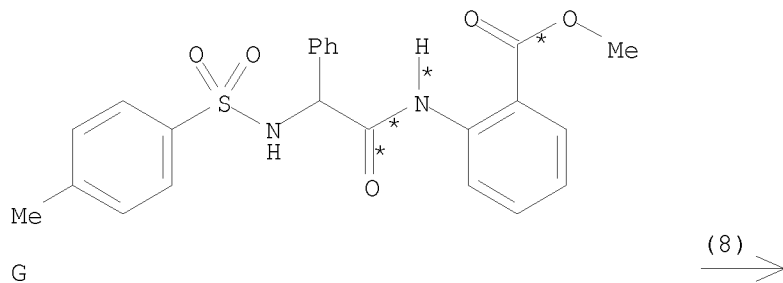
10/ 562,112



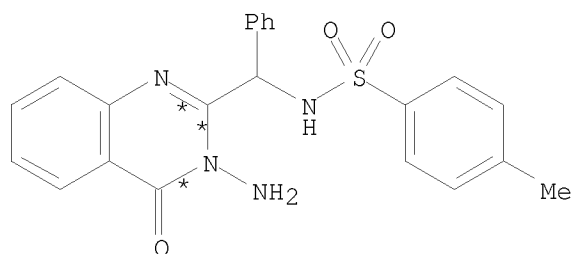
YIELD 74%

RX(7)      RCT   C 351333-19-2  
              RGT   Q 302-01-2 N2H4  
              PRO   P 276687-55-9  
              SOL   7732-18-5 Water, 71-36-3 BuOH

RX(8) OF 76      ...G ==> T



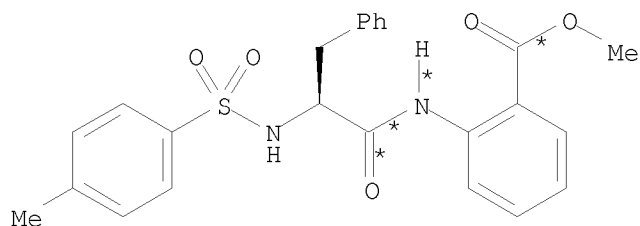
10/ 562,112



T  
YIELD 65%

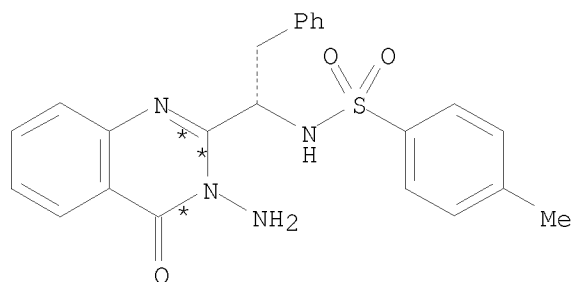
RX(8)      RCT   G 351333-20-5  
             RGT   Q 302-01-2 N<sub>2</sub>H<sub>4</sub>  
             PRO   T 351333-25-0  
             SOL   7732-18-5 Water, 71-36-3 BuOH

RX(9) OF 76      ...I   ==>   U



I

(9) >

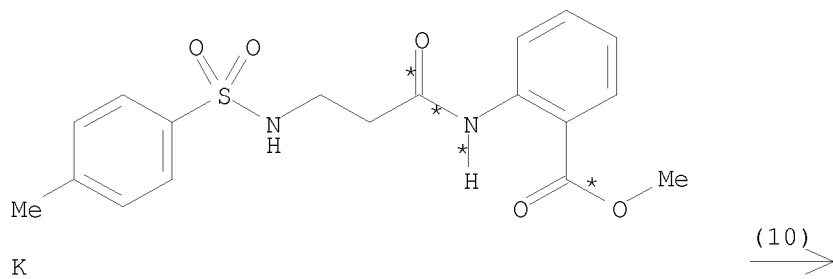


U  
YIELD 68%

RX(9)      RCT   I 351333-21-6  
             RGT   Q 302-01-2 N<sub>2</sub>H<sub>4</sub>  
             PRO   U 351333-26-1  
             SOL   7732-18-5 Water, 71-36-3 BuOH

10/ 562,112

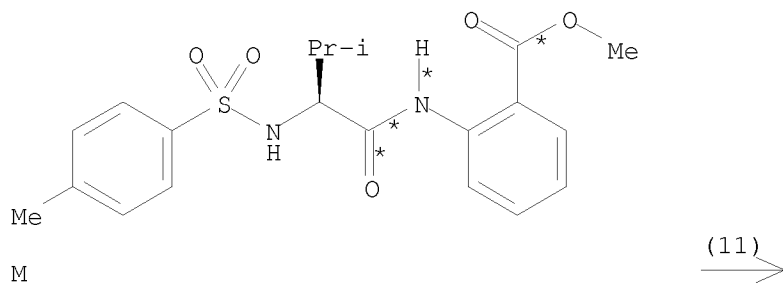
RX(10) OF 76      ...K ==> V...



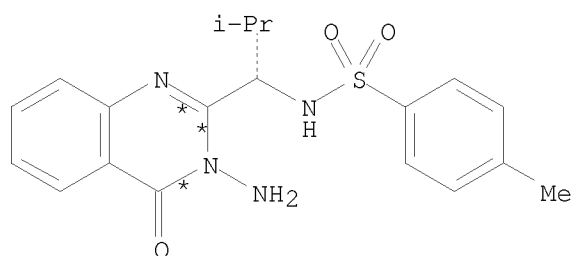
V  
YIELD 70%

RX(10)      RCT    K 351333-22-7  
              RGT    Q 302-01-2 N<sub>2</sub>H<sub>4</sub>  
              PRO    V 351333-27-2  
              SOL    7732-18-5 Water, 71-36-3 BuOH

RX(11) OF 76      ...M ==> W...



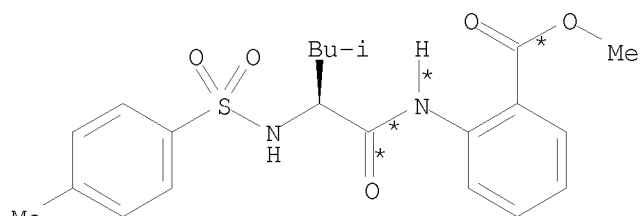
10/ 562,112



W  
YIELD 76%

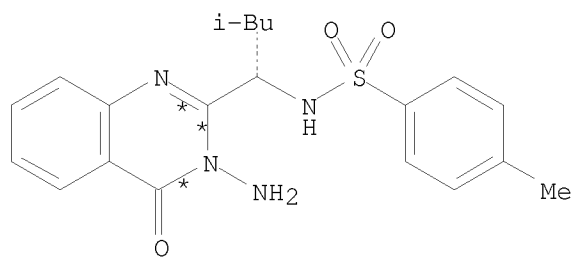
RX(11)     RCT   M 351333-23-8  
              RGT   Q 302-01-2 N2H4  
              PRO   W 351333-28-3  
              SOL   7732-18-5 Water, 71-36-3 BuOH

RX(12) OF 76     ...O   ==>   X



O

(12) >



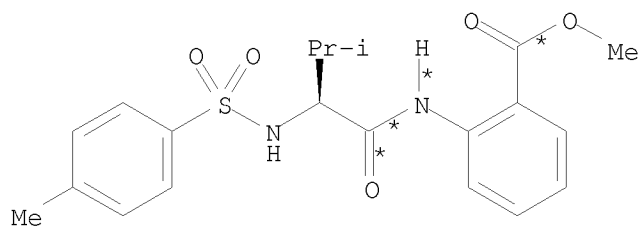
X  
YIELD 71%

RX(12)     RCT   O 351333-24-9  
              RGT   Q 302-01-2 N2H4  
              PRO   X 351333-29-4  
              SOL   7732-18-5 Water, 71-36-3 BuOH

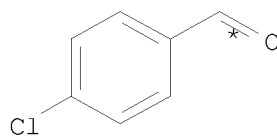


10/ 562,112

RX(40) OF 76 COMPOSED OF RX(11), RX(21)  
RX(40) M + AP ==> AQ

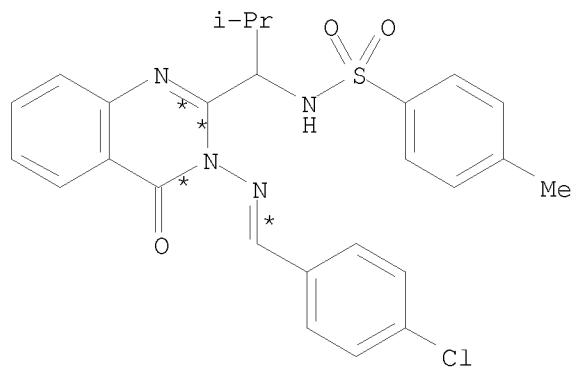


M



AP

2  
STEPS  
=>



AQ  
YIELD 69%

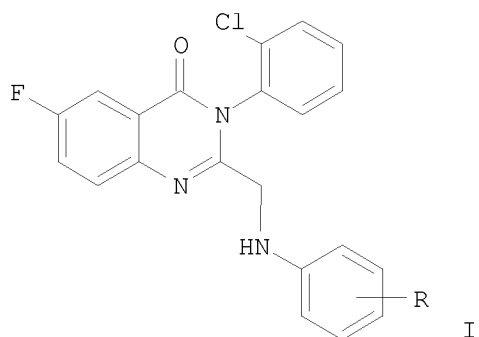
RX(11) RCT M 351333-23-8  
RGT Q 302-01-2 N2H4  
PRO W 351333-28-3  
SOL 7732-18-5 Water, 71-36-3 BuOH

RX(21) RCT W 351333-28-3, AP 104-88-1  
PRO AQ 351333-32-9  
SOL 64-19-7 AcOH

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 106 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 135:76844 CASREACT  
TITLE: Quinazolin-4-one

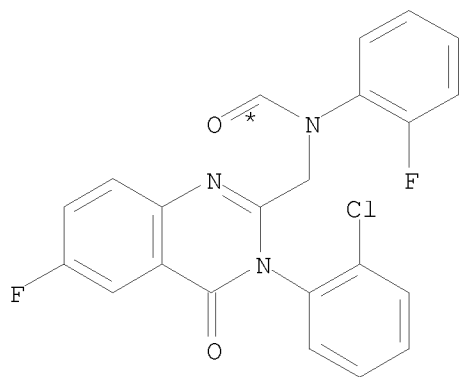
$\alpha$ -Amino-3-hydroxy-5-methyl-4-isoxazolepropionic  
 Acid (AMPA) Receptor Antagonists: Structure-Activity  
 Relationship of the C-2 Side Chain Tether  
 AUTHOR(S): Chenard, Bertrand L.; Welch, Willard M.; Blake, James  
 F.; Butler, Todd W.; Reinhold, Anthony; Ewing, Frank  
 E.; Menniti, Frank S.; Pagnozzi, Martin J.  
 CORPORATE SOURCE: Global Research and Development Groton Laboratories,  
 Pfizer Inc., Groton, CT, 06340, USA  
 SOURCE: Journal of Medicinal Chemistry (2001), 44(11),  
 1710-1717  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB A series of 6-fluoro-3-(2-chlorophenyl)quinazolin-4-ones has been prepared,  
 which contains a 2-fluorophenyl ring attached to C-2 by a variety of  
 two-atom tethers. These compds. were used to probe the structure-activity  
 relationship (SAR) for AMPA receptor inhibition. The relative potencies  
 of the new compds. ranged from 11 nM to greater than 10  $\mu$ M. The  
 differential activity of the compds. was rationalized on the basis of  
 alterations of the 2-fluorophenyl positioning (planar and radial) relative  
 to the quinazolin-4-one ring based on computational methods. From this  
 effort, new AMPA receptor antagonists I [R = 2-F, 2-CN, 3-CN,  
 3-pyrrolidinomethyl], containing the methylamino tether group, have been  
 identified.

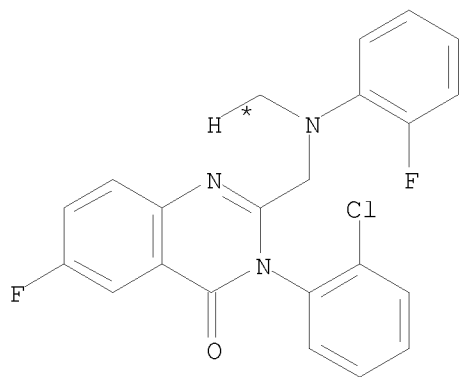
RX(11) OF 53 ...AW ==> AX

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AW

(11)  $\longrightarrow$



AX

YIELD 30%

RX(11) RCT AW 346700-98-9

STAGE(1)

RGT AY 14044-65-6 BH3-THF

SOL 109-99-9 THF

CON 18 hours, room temperature

STAGE(2)

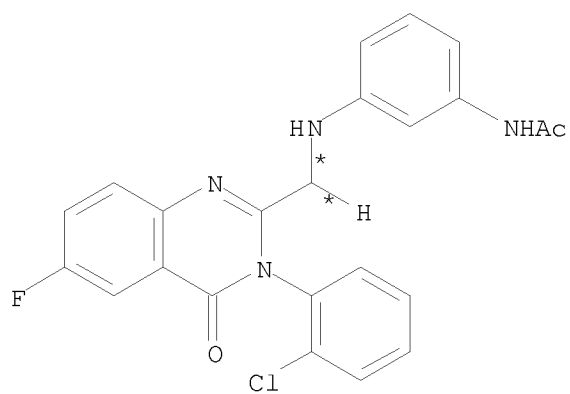
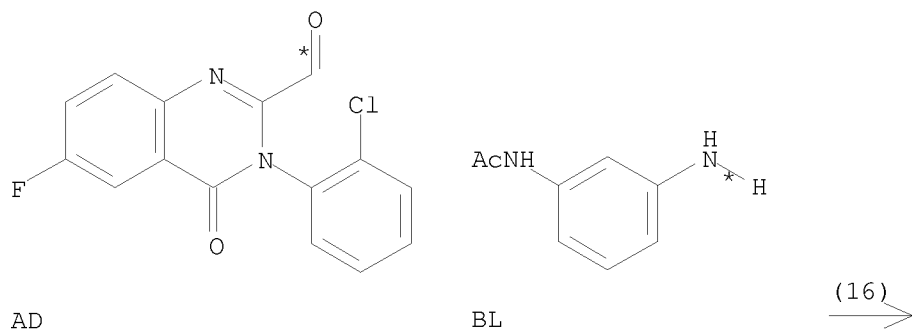
RGT AJ 67-56-1 MeOH

CON room temperature

PRO AX 346700-94-5

RX(16) OF 53 ...AD + BL ==> BM

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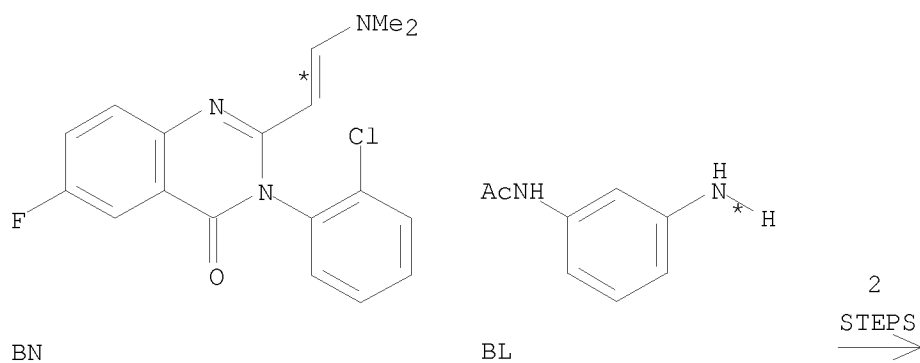


BM  
YIELD 29%

RX(16)     RCT   AD 217942-80-8, BL 102-28-3  
             RGT   AH 56553-60-7 Na.(AcO)3BH  
             PRO   BM 217942-64-8  
             SOL   107-06-2 ClCH2CH2Cl  
             CON   18 hours, room temperature

RX(33) OF 53 COMPOSED OF RX(17), RX(16)  
RX(33)     BN   +   BL   ==>   BM

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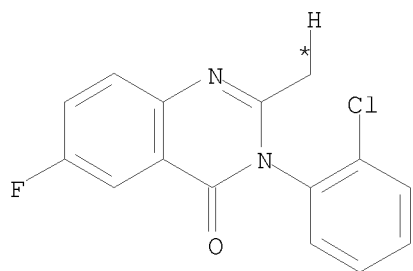


BM  
YIELD 29%

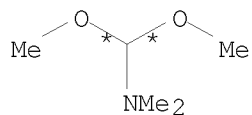
RX(17) RCT BN 217943-01-6  
RGT BO 7790-28-5 NaIO<sub>4</sub>  
PRO AD 217942-80-8  
SOL 7732-18-5 Water, 109-99-9 THF  
CON SUBSTAGE(1) room temperature, pH 7  
SUBSTAGE(2) heated  
SUBSTAGE(3) 1 hour, room temperature  
NTE buffered solution, 1:2 mixture of free aldehyde and hydrate are formed

RX(16) RCT AD 217942-80-8, BL 102-28-3  
RGT AH 56553-60-7 Na.(AcO)3BH  
PRO BM 217942-64-8  
SOL 107-06-2 ClCH<sub>2</sub>CH<sub>2</sub>Cl  
CON 18 hours, room temperature

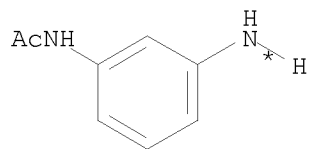
RX(52) OF 53 COMPOSED OF RX(21), RX(17), RX(16)  
RX(52) A + BX + BL ==> BM



A

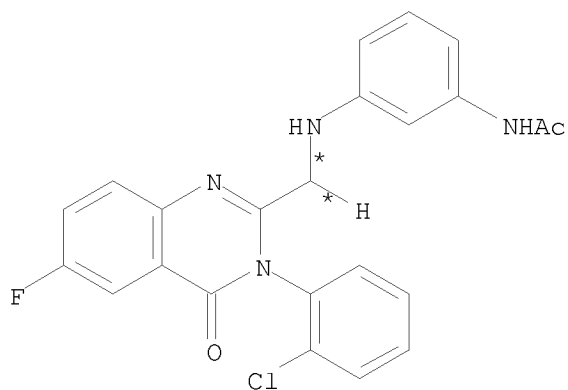


BX



BL

3  
STEPS  
→



BM  
YIELD 29%

RX(21)	RCT	A 49579-12-6, BX 4637-24-5
	PRO	BN 217943-01-6
	SOL	68-12-2 DMF
	CON	SUBSTAGE(1) 24 hours, 140 deg C
		SUBSTAGE(2) 140 deg C -> room temperature
	NTE	thermal
RX(17)	RCT	BN 217943-01-6
	RGT	BO 7790-28-5 NaIO4
	PRO	AD 217942-80-8
	SOL	7732-18-5 Water, 109-99-9 THF
	CON	SUBSTAGE(1) room temperature, pH 7
		SUBSTAGE(2) heated
		SUBSTAGE(3) 1 hour, room temperature
	NTE	buffered solution, 1:2 mixture of free aldehyde and hydrate are formed
RX(16)	RCT	AD 217942-80-8, BL 102-28-3

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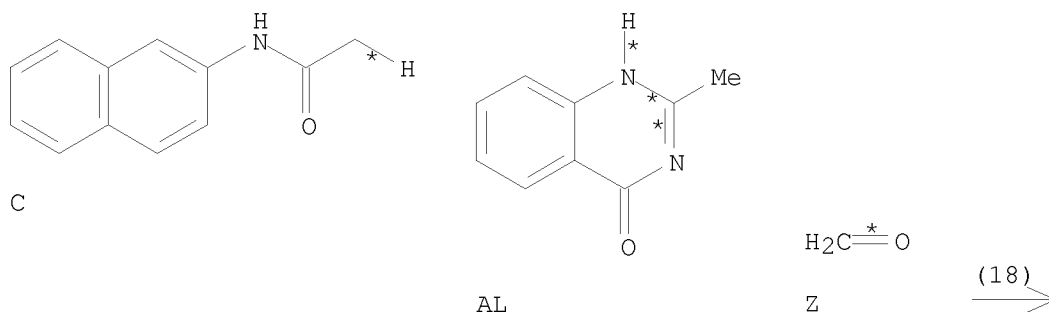
RGT AH 56553-60-7 Na.(AcO)3BH  
PRO BM 217942-64-8  
SOL 107-06-2 ClCH2CH2Cl  
CON 18 hours, room temperature

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

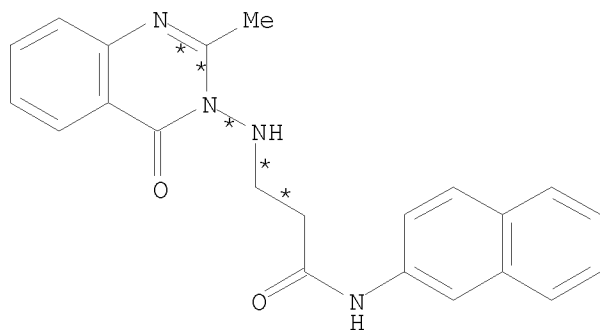
L3 ANSWER 107 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 135:33439 CASREACT  
TITLE: Synthesis and anti-inflammatory activity of  
1-acetyl-5-(substituted  
aryl)-3-( $\beta$ -naphthylamino)-2-pyrazolines and  
[(substituted  $\beta$ -aminoethyl)amido]naphthalenes  
AUTHOR(S): Bansal, Ekta; Srivastava, V. K.; Kumar, Ashok  
CORPORATE SOURCE: Medicinal Chemistry Division, Department of  
Pharmacology, L.L.R.M. Medical College, Meerut,  
250004, India  
SOURCE: European Journal of Medicinal Chemistry (2001), 36(1),  
81-92  
CODEN: EJMCA5; ISSN: 0223-5234  
PUBLISHER: Editions Scientifiques et Medicales Elsevier  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The title compds. were prepared by reaction of  
 $\beta$ -(acetylamino)naphthalene with aromatic aldehydes followed by  
cyclization with N2H4.H2O or by reaction with primary or secondary amines  
(Mannich reaction), resp. The structures of new compds. were confirmed by  
1H-NMR and IR. Anti-inflammatory and ulcerogenic activities in vivo were  
evaluated and compared with the standard drugs phenylbutazone and  
indomethacin. Some compds. of the series exhibited promising  
anti-inflammatory activity with a lower ulcerogenic liability than the  
standard drugs.

RX(18) OF 66 ...C + AL + Z ==> AM



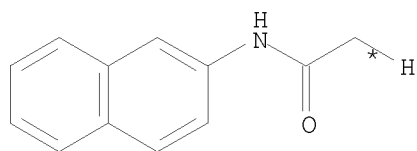
10/ 562,112



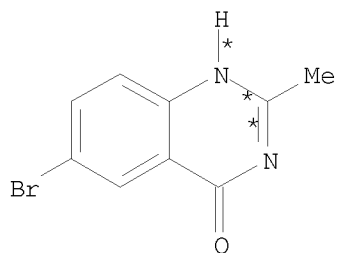
AM  
YIELD 40%

RX(18)      RCT   C 581-97-5, AL 1769-24-0, Z 50-00-0  
               RGT   T 302-01-2 N2H4  
               PRO   AM 343930-76-7  
               SOL   64-17-5 EtOH

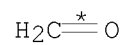
RX(19) OF 66      ...C + AN + Z ==> AO



C



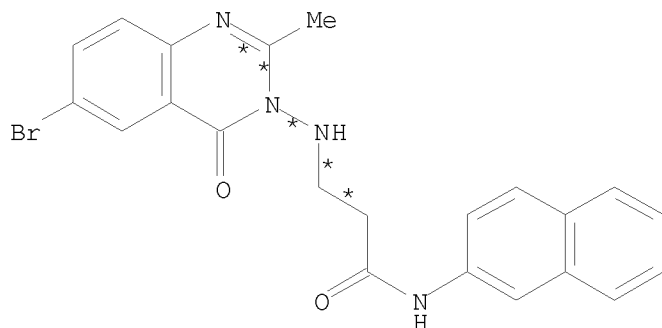
AN



Z

(19) →





AO  
YIELD 55%

RX(19) RCT C 581-97-5, AN 5426-59-5, Z 50-00-0  
RGT T 302-01-2 N2H4  
PRO AO 343930-77-8  
SOL 64-17-5 EtOH

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 108 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 134:222305 CASREACT

TITLE: Stereoisomerism in  
3-[N-(2-acetoxypropanoyl)-N-acylamino]quinazolin-4(3H)-ones, enantioselective acylating agents

AUTHOR(S): Al-Sehemi, Abdullah G.; Atkinson, Robert S.; Fawcett, John; Russell, David R.

CORPORATE SOURCE: Department of Chemistry, Leicester University, Leicester, LE1 7RH, UK

SOURCE: Perkin 1 (2000), (24), 4413-4421  
CODEN: PERKF9; ISSN: 1470-4358

PUBLISHER: Royal Society of Chemistry

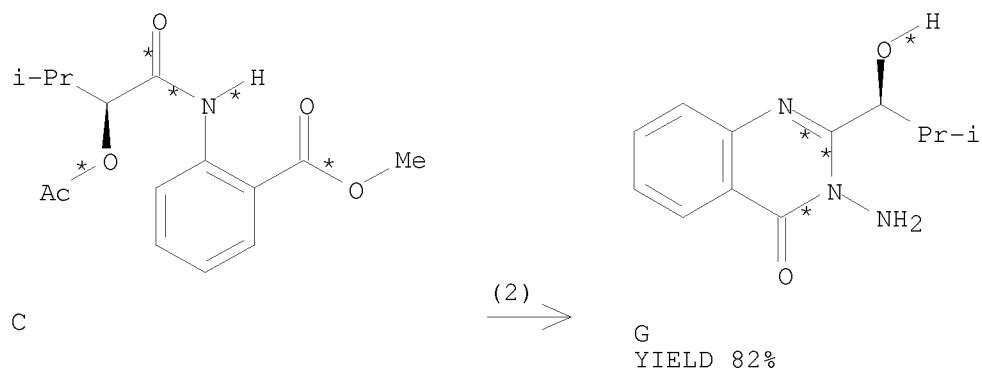
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The title compds. diacylaminoquinazolinones (DAQs) are enantioselective acylation agents for amines and a detailed study of their stereostructures was undertaken with the aim of understanding how this enantioselectivity arises. The N-N bond in these DAQs is a chiral axis. Even where both N-acyl groups are (S)-2-acetoxypropanoyl, the N-N bond is still a chiral axis because in the most stable conformation of the planar imide moiety, one exo/endo orientation of the carbonyl groups is much preferred over the alternative (endo/exo) as revealed by NMR spectroscopy. A conformational preference within the 2-acetoxypropanoyl grouping accounts for the presence of a single exo/endo conformation in solution for some of these DAQs (see above) but an interconverting exo/endo .dblharw. endo/exo mixture for others. Where a single exo/endo conformation is present in solution, evidence is presented that this closely resembles the X-ray determined crystal structure. A mechanism for the second acylation step to form these DAQs is proposed, which involves preliminary O-acylation of the 3-(monoacylamino)quinazolinone.

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RX(2) OF 18      ...C ==> G...



RX(2)      RCT   C 329729-34-2

STAGE(1)

RGT   H 302-01-2 N2H4

SOL   64-17-5 EtOH

STAGE(2)

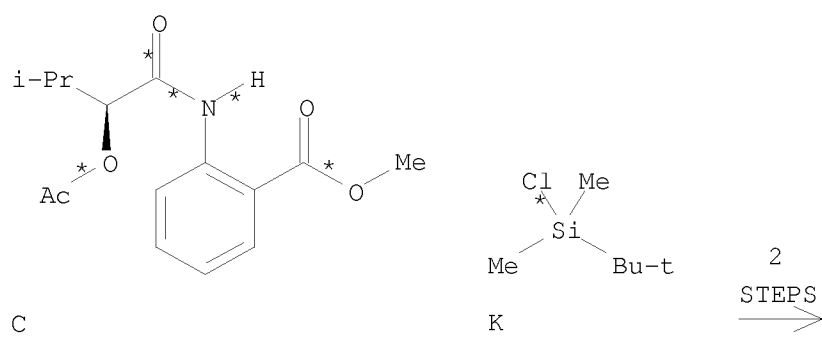
SOL   75-09-2 CH2Cl2

PRO   G 329729-35-3

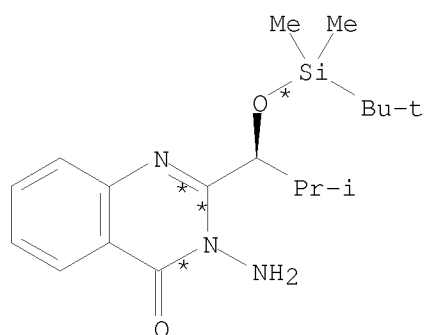
NTE   stereoselective

RX(10) OF 18 COMPOSED OF RX(2), RX(3)

RX(10)      C + K ==> L



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L  
YIELD 96%

RX(2) RCT C 329729-34-2

STAGE(1)

RGT H 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 75-09-2 CH2Cl2

PRO G 329729-35-3

NTE stereoselective

RX(3) RCT G 329729-35-3, K 18162-48-6

RGT M 288-32-4 1H-Imidazole

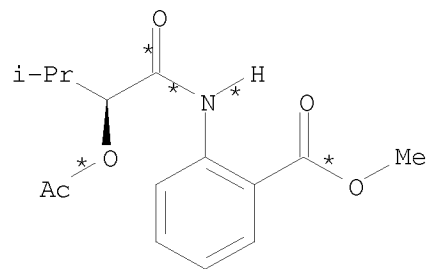
PRO L 262600-86-2

SOL 68-12-2 DMF

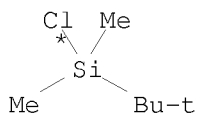
NTE stereoselective

RX(15) OF 18 COMPOSED OF RX(2), RX(3), RX(4)

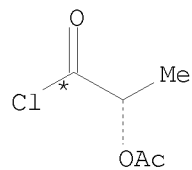
RX(15) C + K + N ==> O



C



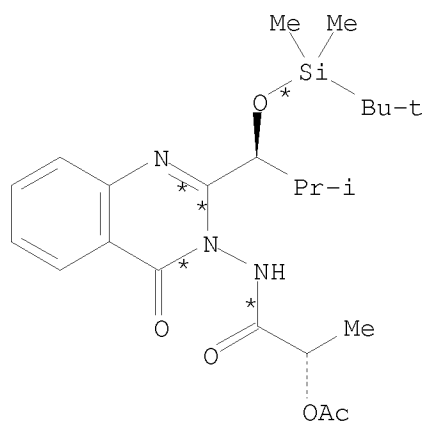
K



N

3  
STEPS  
→

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O  
YIELD 88%

RX(2) RCT C 329729-34-2

STAGE(1)

RGT H 302-01-2 N2H4  
SOL 64-17-5 EtOH

STAGE(2)

SOL 75-09-2 CH2Cl2

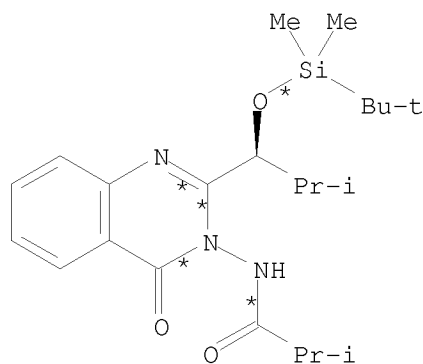
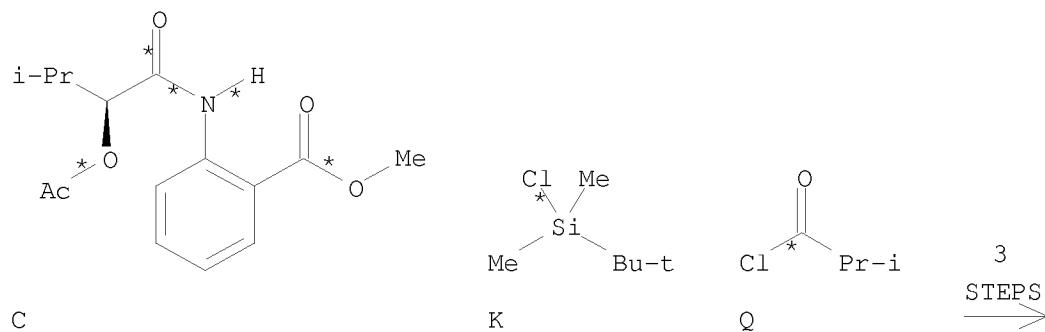
PRO G 329729-35-3  
NTE stereoselective

RX(3) RCT G 329729-35-3, K 18162-48-6  
RGT M 288-32-4 1H-Imidazole  
PRO L 262600-86-2  
SOL 68-12-2 DMF  
NTE stereoselective

RX(4) RCT L 262600-86-2, N 36394-75-9  
RGT P 110-86-1 Pyridine  
PRO O 329729-36-4  
SOL 75-09-2 CH2Cl2  
NTE stereoselective

RX(16) OF 18 COMPOSED OF RX(2), RX(3), RX(5)  
RX(16) C + K + Q ==> R

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R  
YIELD 79%

RX(2) RCT C 329729-34-2

STAGE(1)

RGT H 302-01-2 N2H4  
SOL 64-17-5 EtOH

STAGE(2)

SOL 75-09-2 CH2Cl2

PRO G 329729-35-3  
NTE stereoselective

RX(3) RCT G 329729-35-3, K 18162-48-6  
RGT M 288-32-4 1H-Imidazole  
PRO L 262600-86-2  
SOL 68-12-2 DMF  
NTE stereoselective

RX(5) RCT L 262600-86-2, Q 79-30-1  
RGT P 110-86-1 Pyridine  
PRO R 262600-88-4  
SOL 75-09-2 CH2Cl2  
NTE stereoselective

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 109 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 134:157195 CASREACT

TITLE: Synthesis and antifungal activity of some new quinazoline and benzoxazinone derivatives

AUTHOR(S): Shalaby, Alyaa A.; El-Khamry, Abdel Momen A.; Shiba, S. A.; Ahmed, Abdel Aal Alm Eldeen Abdalah; Hanafi, Awaref A.

CORPORATE SOURCE: Chemistry Department, Faculty of Science, Ain Shams University, Cairo, Egypt

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2000), 333(11), 365-372

CODEN: ARPMAS; ISSN: 0365-6233

PUBLISHER: Wiley-VCH Verlag GmbH

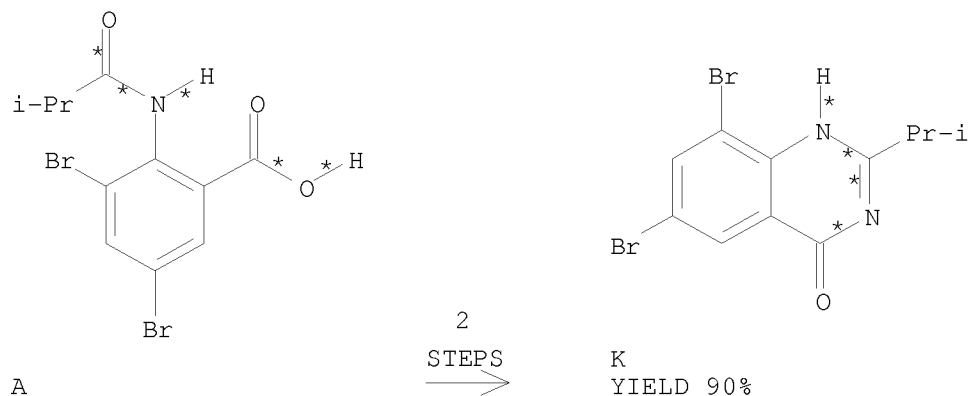
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The hitherto unknown 2-isopropyl-6,8-dibromo-4H-3,1-benzoxazin-4-one was subjected to condensation with either primary or secondary amines affording the benzamide derivs., while with alcs. in presence of the base, corresponding esters were obtained. A series of other compds. were also prepared according to the methods discussed in the text. Ten of our compds. were examined against *Sclerotium cepivorum* as well as *Botrytis allii* on PDA media. These compds. showed a significant reduction of mycelial growth and sclerotia number of these fungi which cause the white rot and neck rot diseases of onion.

RX(34) OF 113 COMPOSED OF RX(1), RX(5)

RX(34) A ==> K



RX(1) RCT A 325707-07-1  
PRO B 325707-08-2  
SOL 108-24-7 Ac2O  
NTE PETROLEUM USED

RX(5) RCT B 325707-08-2

STAGE(1)

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RGT L 631-61-8 NH4OAc

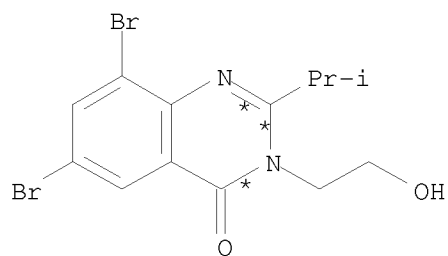
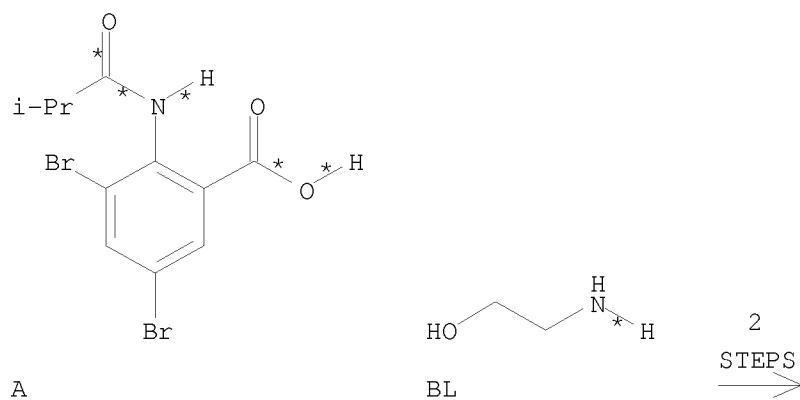
STAGE(2)

SOL 7732-18-5 Water

PRO K 325707-24-2

RX(39) OF 113 COMPOSED OF RX(1), RX(28)

RX(39) A + BL ==> N



N  
YIELD 60%

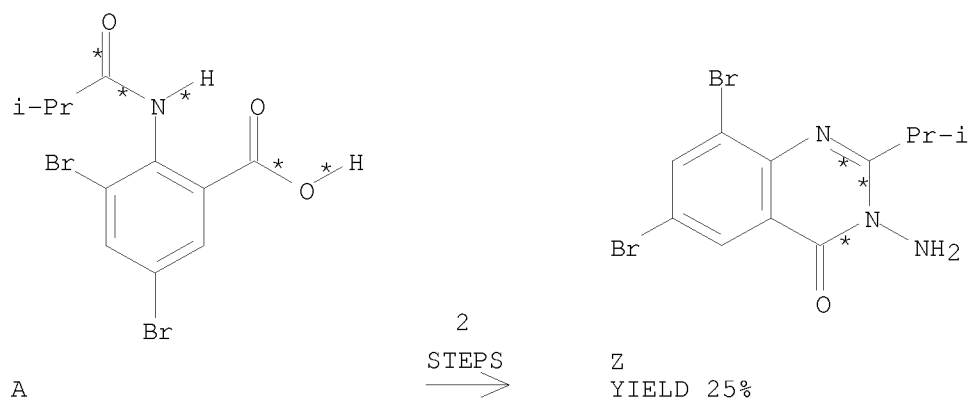
RX(1) RCT A 325707-07-1  
PRO B 325707-08-2  
SOL 108-24-7 Ac2O  
NTE PETROLEUM USED

RX(28) RCT B 325707-08-2, BL 141-43-5  
PRO N 325707-16-2  
NTE PETROLEUM USED

RX(40) OF 113 COMPOSED OF RX(1), RX(29)

RX(40) A ==> Z

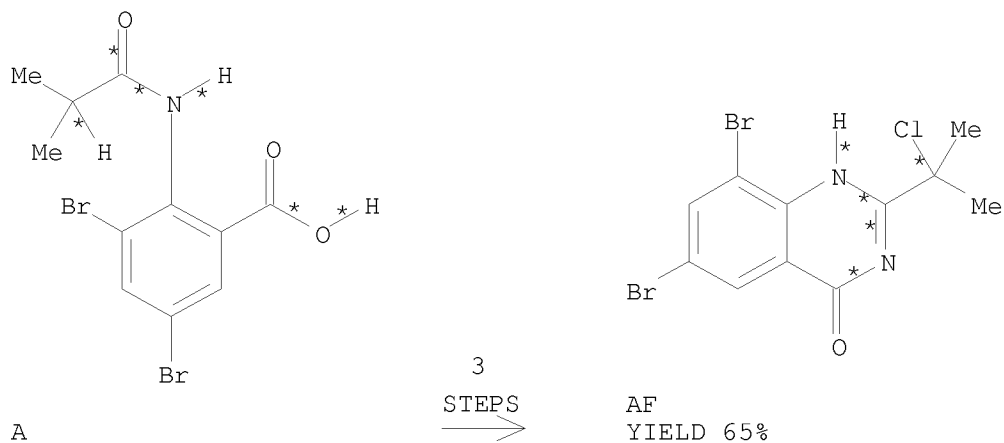
10/ 562,112



RX(1) RCT A 325707-07-1  
PRO B 325707-08-2  
SOL 108-24-7 Ac2O  
NTE PETROLEUM USED

RX(29) RCT B 325707-08-2  
RGT BM 7803-57-8 N2H4-H2O  
PRO Z 325707-19-5  
SOL 64-17-5 EtOH

RX(59) OF 113 COMPOSED OF RX(1), RX(5), RX(13)  
RX(59) A ==> AF



RX(1) RCT A 325707-07-1  
PRO B 325707-08-2  
SOL 108-24-7 Ac2O  
NTE PETROLEUM USED

RX(5) RCT B 325707-08-2

STAGE(1)  
RGT L 631-61-8 NH4OAc



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STAGE(2)

SOL 7732-18-5 Water

PRO K 325707-24-2

RX(13) RCT K 325707-24-2

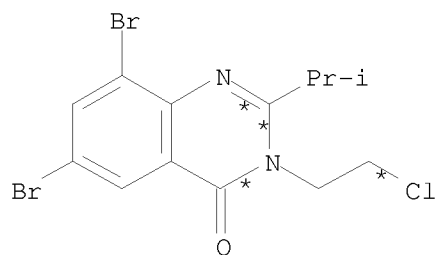
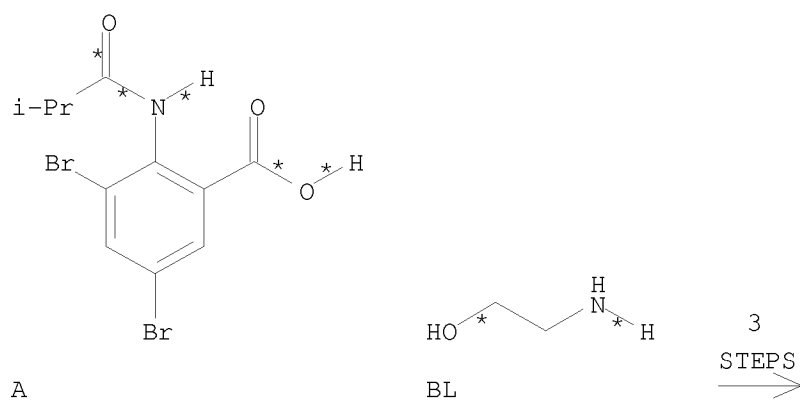
RGT AG 10025-87-3 POC13, AH 10026-13-8 PC15

PRO AF 325707-36-6

SOL 108-88-3 PhMe

RX(60) OF 113 COMPOSED OF RX(1), RX(28), RX(6)

RX(60) A + BL ==> O



O  
YIELD 70%

RX(1) RCT A 325707-07-1  
PRO B 325707-08-2  
SOL 108-24-7 Ac2O  
NTE PETROLEUM USED

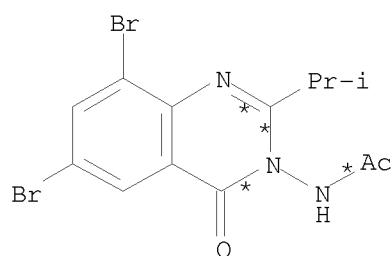
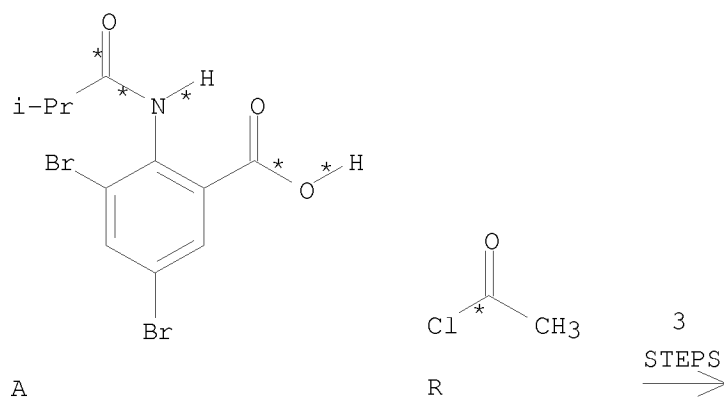
RX(28) RCT B 325707-08-2, BL 141-43-5  
PRO N 325707-16-2  
NTE PETROLEUM USED

RX(6) RCT N 325707-16-2  
RGT P 7719-09-7 SOC12

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PRO O 325707-17-3

RX(61) OF 113 COMPOSED OF RX(1), RX(29), RX(10)  
RX(61) A + R ==> AA



AA  
YIELD 65%

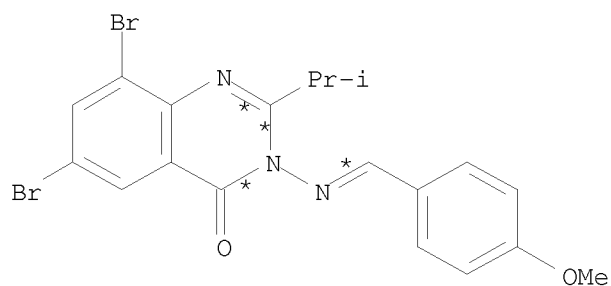
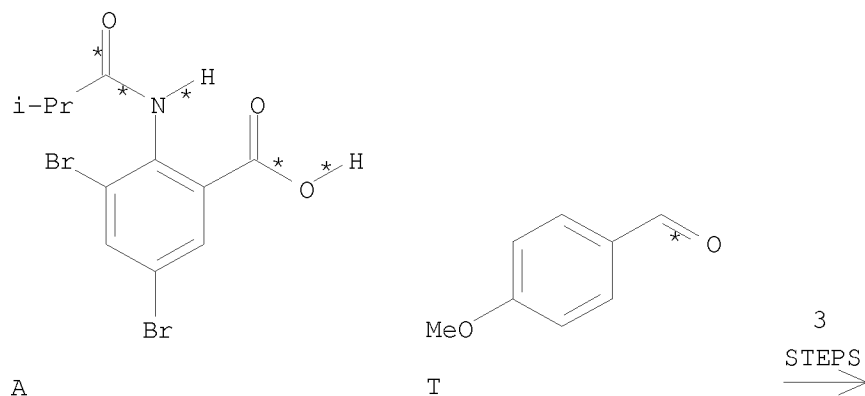
RX(1) RCT A 325707-07-1  
PRO B 325707-08-2  
SOL 108-24-7 Ac2O  
NTE PETROLEUM USED

RX(29) RCT B 325707-08-2  
RGT BM 7803-57-8 N2H4-H2O  
PRO Z 325707-19-5  
SOL 64-17-5 EtOH

RX(10) RCT Z 325707-19-5, R 75-36-5  
PRO AA 325707-21-9

RX(62) OF 113 COMPOSED OF RX(1), RX(29), RX(11)  
RX(62) A + T ==> AB

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AB  
YIELD 75%

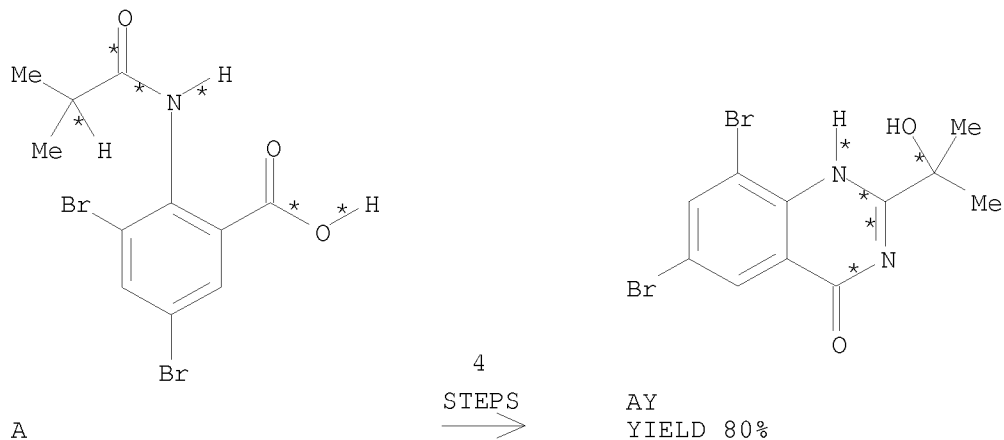
RX(1) RCT A 325707-07-1  
PRO B 325707-08-2  
SOL 108-24-7 Ac2O  
NTE PETROLEUM USED

RX(29) RCT B 325707-08-2  
RGT BM 7803-57-8 N2H4-H2O  
PRO Z 325707-19-5  
SOL 64-17-5 EtOH

RX(11) RCT Z 325707-19-5, T 123-11-5  
PRO AB 325707-23-1  
SOL 64-17-5 EtOH

RX(85) OF 113 COMPOSED OF RX(1), RX(5), RX(13), RX(22)  
RX(85) A ==> AY

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RX(1) RCT A 325707-07-1  
PRO B 325707-08-2  
SOL 108-24-7 Ac2O  
NTE PETROLEUM USED

RX(5) RCT B 325707-08-2  
STAGE(1)  
RGT L 631-61-8 NH4OAc

STAGE(2)  
SOL 7732-18-5 Water

PRO K 325707-24-2

RX(13) RCT K 325707-24-2  
RGT AG 10025-87-3 POC13, AH 10026-13-8 PC15  
PRO AF 325707-36-6  
SOL 108-88-3 PhMe

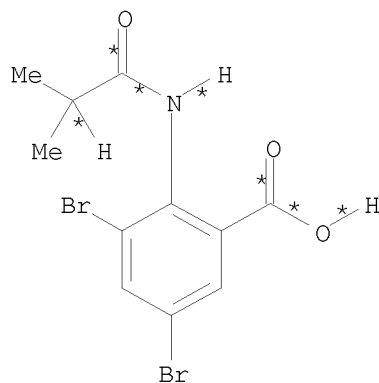
RX(22) RCT AF 325707-36-6  
STAGE(1)  
RGT AL 497-19-8 Na2CO3  
SOL 7732-18-5 Water

STAGE(2)  
RGT AZ 7697-37-2 HNO3

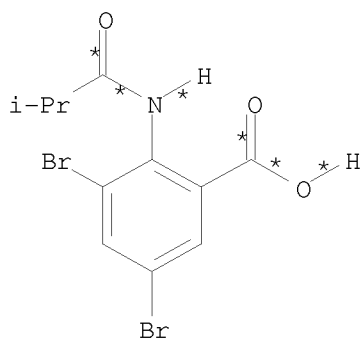
PRO AY 325707-37-7

RX(100) OF 113 COMPOSED OF RX(1), RX(5), RX(12), RX(19), RX(20)  
RX(100) 2 A ==> AF

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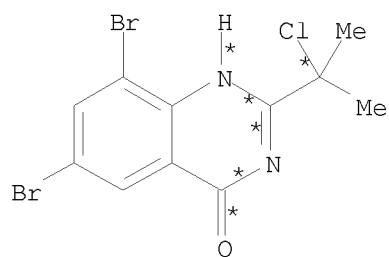


A



A

5  
STEPS  
→



AF  
YIELD 80%

RX(1) RCT A 325707-07-1  
PRO B 325707-08-2  
SOL 108-24-7 Ac2O  
NTE PETROLEUM USED

RX(5) RCT B 325707-08-2

STAGE(1)  
RGT L 631-61-8 NH4OAc

STAGE(2)  
SOL 7732-18-5 Water

PRO K 325707-24-2

RX(12) RCT K 325707-24-2  
RGT AD 19172-47-5 Lawesson's reagent  
PRO AC 325707-26-4  
SOL 108-88-3 PhMe

RX(19) RCT AC 325707-26-4  
RGT AG 10025-87-3 POC13, AH 10026-13-8 PC15  
PRO AU 325707-34-4, AV 325707-35-5

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RX(20) RCT AV 325707-35-5

STAGE(1)

RGT AW 26628-22-8 NaN3

SOL 64-19-7 AcOH

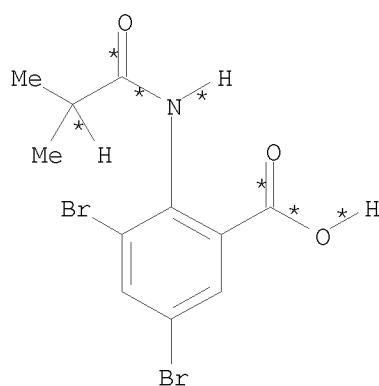
STAGE(2)

SOL 7732-18-5 Water

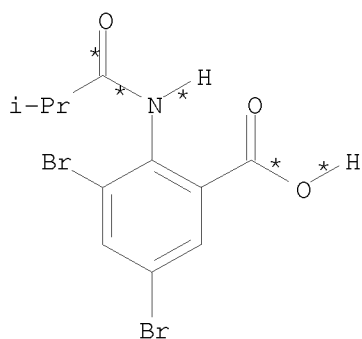
PRO AF 325707-36-6

RX(112) OF 113 COMPOSED OF RX(1), RX(5), RX(12), RX(19), RX(20), RX(22)

RX(112) 2 A ==> AY

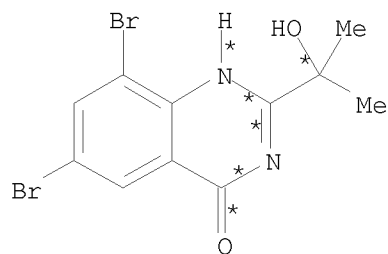


A



A

6  
STEPS  
→



AY

YIELD 80%

RX(1) RCT A 325707-07-1  
PRO B 325707-08-2  
SOL 108-24-7 Ac2O  
NTE PETROLEUM USED

RX(5) RCT B 325707-08-2

STAGE(1)

RGT L 631-61-8 NH4OAc

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STAGE(2)  
SOL 7732-18-5 Water

PRO K 325707-24-2

RX(12) RCT K 325707-24-2  
RGT AD 19172-47-5 Lawesson's reagent  
PRO AC 325707-26-4  
SOL 108-88-3 PhMe

RX(19) RCT AC 325707-26-4  
RGT AG 10025-87-3 POC13, AH 10026-13-8 PC15  
PRO AU 325707-34-4, AV 325707-35-5

RX(20) RCT AV 325707-35-5

STAGE(1)  
RGT AW 26628-22-8 NaN3  
SOL 64-19-7 AcOH

STAGE(2)  
SOL 7732-18-5 Water

PRO AF 325707-36-6

RX(22) RCT AF 325707-36-6

STAGE(1)  
RGT AL 497-19-8 Na2CO3  
SOL 7732-18-5 Water

STAGE(2)  
RGT AZ 7697-37-2 HNO3

PRO AY 325707-37-7

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 110 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 134:100515 CASREACT

TITLE: Tetraacyl hydrazines and  
3,3'-biquinazoline-4,4'-diones; synthesis, studies of  
rotational barriers and deracemisation

AUTHOR(S): Coogan, Michael P.; Passey, Steven C.

CORPORATE SOURCE: Science Laboratories, Department of Chemistry,  
University of Durham, Durham, DH1 3LE, UK

SOURCE: Perkin 2 (2000), (10), 2060-2066

CODEN: PRKTFO; ISSN: 1470-1820

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

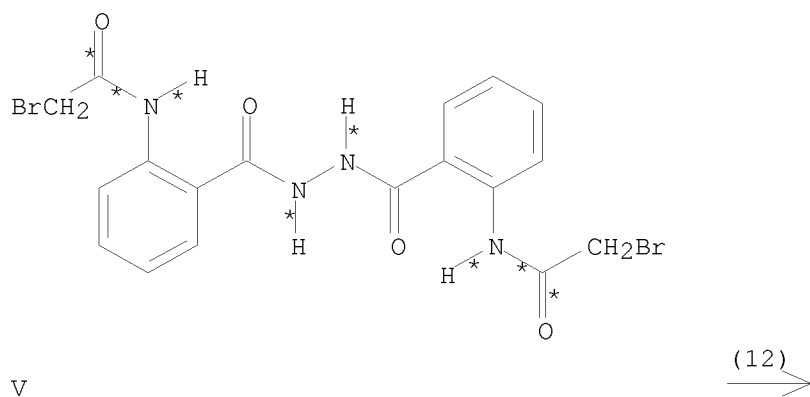
LANGUAGE: English

AB The barrier to rotation around the N-N bond in  
3,3'-biquinazoline-4,4'-dione is estimated to be 96 kJ mol<sup>-1</sup>, significantly  
higher than in acyclic tetraacyl hydrazines (84 kJ mol<sup>-1</sup>). Both dynamic  
chiroptical and NMR studies of 3,3'-biquinazoline-4,4'-diones which have

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an addnl. ring bridging the 2,2' positions indicate that these compds. have a significantly higher barrier to rotation than the parent 3,3'-biquinazoline-4,4'-dione. Deracemization of certain 3,3'-biquinazoline-4,4'-diones is possible via treatment with chiral acids at high temperature

RX(12) OF 34 ...V ==> AE...



AE  
YIELD 81%

RX(12) RCT V 319426-05-6

STAGE(1)

RGT AM 104-15-4 TsOH

SOL 108-88-3 PhMe

STAGE(2)

SOL 141-78-6 AcOEt

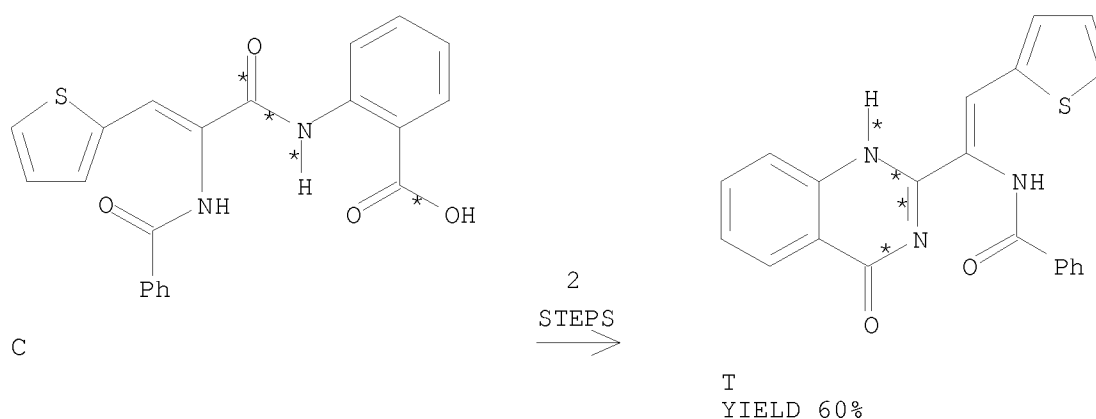
PRO AE 253141-07-0

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



ACCESSION NUMBER: 134:86206 CASREACT  
 TITLE: The behaviour of some nucleophiles towards  
 2-[ $\alpha$ -(benzoylamino)- $\beta$ -(2-thienyl)vinyl]benzoxazin-4(3H)-one  
 AUTHOR(S): Guirguis, Dalal B.  
 CORPORATE SOURCE: Chemistry Department, Faculty of Science, Ain Shams  
 University, Cairo, Egypt  
 SOURCE: Indian Journal of Chemistry, Section B: Organic  
 Chemistry Including Medicinal Chemistry (2000),  
 39B(4), 264-269  
 CODEN: IJSBDB; ISSN: 0376-4699  
 PUBLISHER: National Institute of Science Communication, CSIR  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB 2-[ $\alpha$ -(Benzoylamino)- $\beta$ -thien-2-ylvinyl]benzoxazin-4(3H)-one (I)  
 undergoes ring-opening on treatment with primary and secondary amines  
 affording 2-[ $\alpha$ -(benzoylamino)- $\beta$ -thien-2-ylacrylamido]benzamides. Treatment of I with HCONH<sub>2</sub> and N<sub>2</sub>H<sub>4</sub>.H<sub>2</sub>O at  
 elevated temperature gives rise to quinazolinones. Interestingly, reaction of  
 vicinal aminobenzyl alcs. with I yields the usual ring-opening products  
 and unexpected 4-iminobenzoxazines.

RX(29) OF 80 COMPOSED OF RX(2), RX(9)  
 RX(29) C ==> T



RX(2) RCT C 318292-63-6  
 STAGE(1)  
 SOL 108-24-7 Ac<sub>2</sub>O  
 STAGE(2)  
 SOL 7732-18-5 Water  
 PRO F 318292-64-7  
 RX(9) RCT F 318292-64-7  
 STAGE(1)  
 RGT U 75-12-7 Formamide  
 SOL 64-17-5 EtOH

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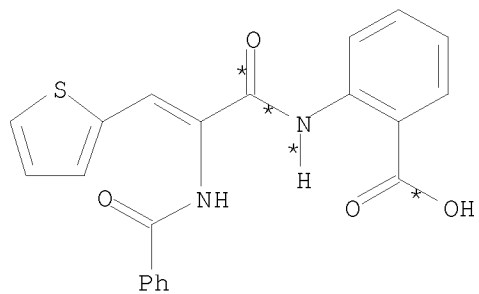
STAGE(2)

SOL 7732-18-5 Water

PRO T 318292-72-7

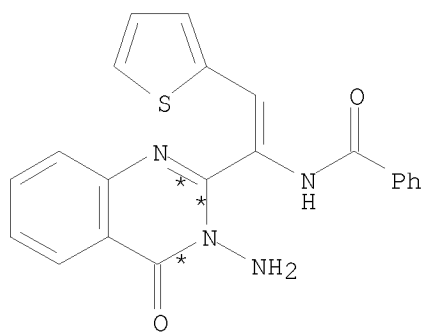
RX(30) OF 80 COMPOSED OF RX(2), RX(10)

RX(30) C ==> V



C

2  
STEPS  
→



V

YIELD 60%

RX(2) RCT C 318292-63-6

STAGE(1)

SOL 108-24-7 Ac2O

STAGE(2)

SOL 7732-18-5 Water

PRO F 318292-64-7

RX(10) RCT F 318292-64-7

RGT I 302-01-2 N2H4

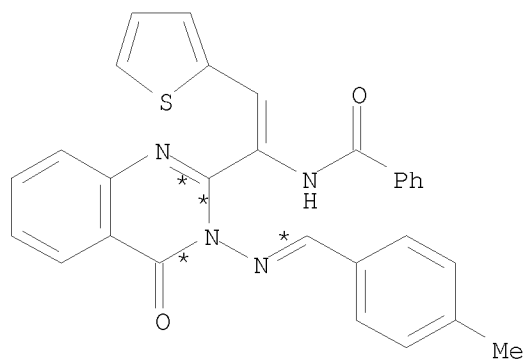
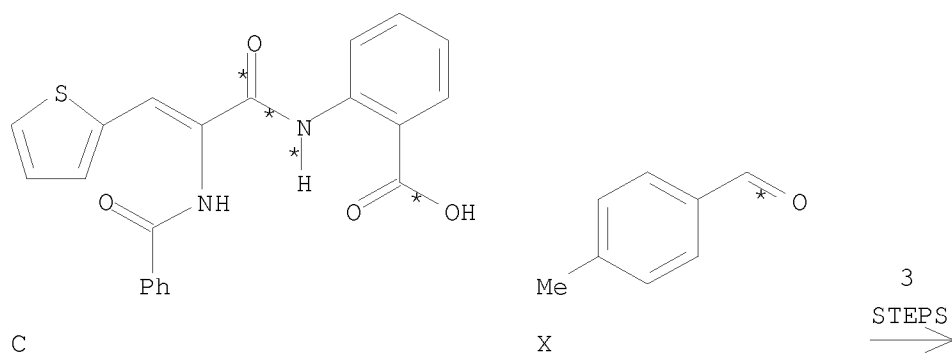
PRO V 318292-73-8

SOL 71-36-3 BuOH

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RX(74) OF 80 COMPOSED OF RX(2), RX(10), RX(11)

RX(74) C + X ==> Y



Y  
YIELD 40%

RX(2) RCT C 318292-63-6

STAGE(1)

SOL 108-24-7 Ac2O

STAGE(2)

SOL 7732-18-5 Water

PRO F 318292-64-7

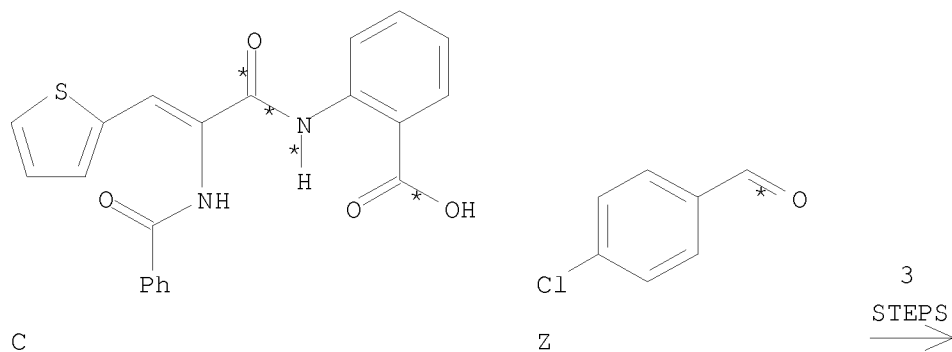
RX(10) RCT F 318292-64-7  
RGT I 302-01-2 N2H4  
PRO V 318292-73-8  
SOL 71-36-3 BuOH

RX(11) RCT V 318292-73-8, X 104-87-0  
PRO Y 318292-74-9  
CAT 110-89-4 Piperidine  
SOL 64-17-5 EtOH

RX(75) OF 80 COMPOSED OF RX(2), RX(10), RX(12)

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RX(75)      C   +   Z   ==>   AA



AA  
YIELD 48%

RX(2)      RCT   C 318292-63-6

STAGE(1)

SOL 108-24-7 Ac2O

STAGE(2)

SOL 7732-18-5 Water

PRO   F 318292-64-7

RX(10)      RCT   F 318292-64-7  
RGT   I 302-01-2 N2H4  
PRO   V 318292-73-8  
SOL   71-36-3 BuOH

RX(12)      RCT   V 318292-73-8, Z 104-88-1  
PRO   AA 318292-75-0  
CAT   110-89-4 Piperidine  
SOL   64-17-5 EtOH

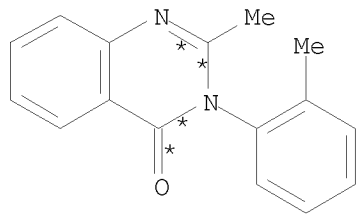
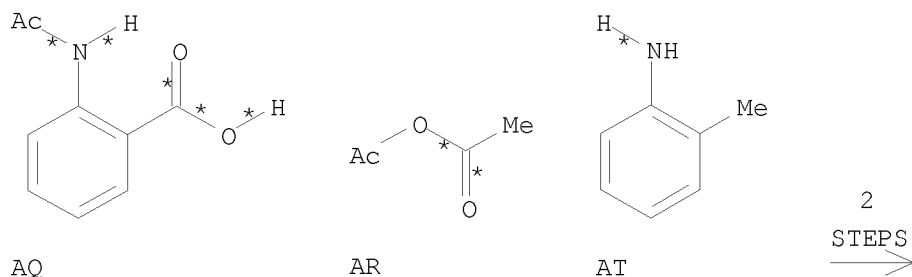
REFERENCE COUNT:      16      THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 112 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 134:72897 CASREACT  
 TITLE: Synthesis of 2-methyl-3-(2'-methylphenyl)-6-aryl  
 azo-4-oxoquinazoline derivatives and their application  
 AUTHOR(S): Patel, R. B.; Patel, Nilesh; Patel, S. K.; Patel, K.  
 C.  
 CORPORATE SOURCE: Department of Chemistry, South Gujarat University,  
 Surat, 395 007, India  
 SOURCE: Oriental Journal of Chemistry (2000), 16(2), 305-310  
 CODEN: OJCHEG; ISSN: 0970-020X  
 PUBLISHER: Oriental Scientific Publishing Co.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A series of dyes has been prepared by coupling of diazotized  
 2-methyl-3-(2-methylphenyl)-6-amino-4-oxoquinazoline with various coupling  
 components to give 4-oxoquinazoline-based azo dyes and their dyeing  
 performance on silk, wool, and rayon has been assessed. These dyes have  
 been found to give a variety of color shades with very good depth and  
 levelness on the fibers. The IR spectra showed all characteristic bands  
 and a representative dye PMR spectrum showed all the expected signals.  
 The percentage dye-bath exhaustion and fixation on different fibers was  
 reasonably good and acceptable, resp. The dyed fibers showed good to  
 excellent fastness to light, washing, and rubbing.

RX(22) OF 95 COMPOSED OF RX(18), RX(19)

RX(22) AQ + AR + AT ==> AU



AU  
 YIELD 89%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
 PRO AS 525-76-8

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RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

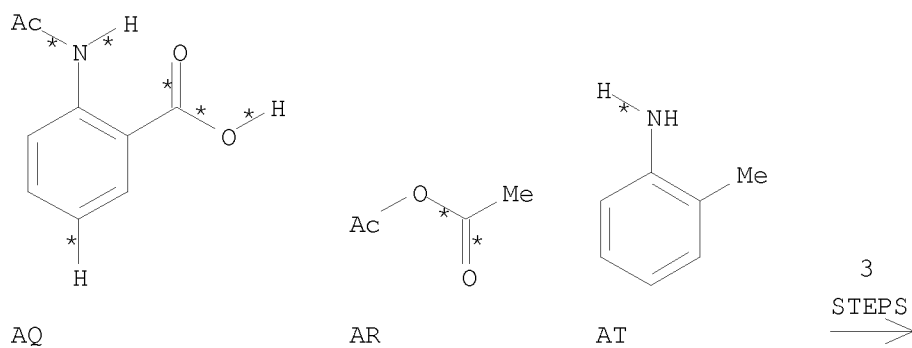
STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(42) OF 95 COMPOSED OF RX(18), RX(19), RX(20)

RX(42) AQ + AR + AT ==> AV



AV  
YIELD 95%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

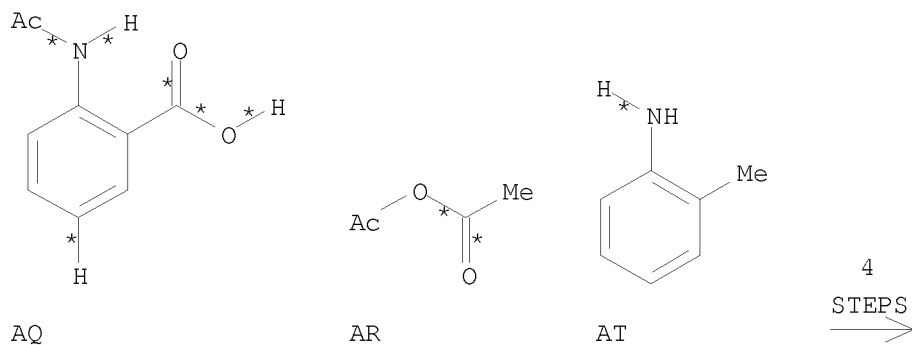
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STAGE(2)  
SOL 7732-18-5 Water

STAGE(3)  
RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(44) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21)  
RX(44) AQ + AR + AT ==> A



A  
YIELD 88%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)  
RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)  
RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

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SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

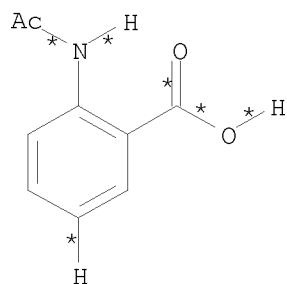
RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

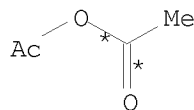
PRO A 963-34-8

RX(79) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(1)

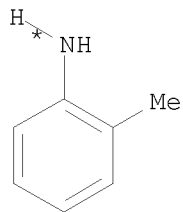
RX(79) AQ + AR + AT + B ==> C



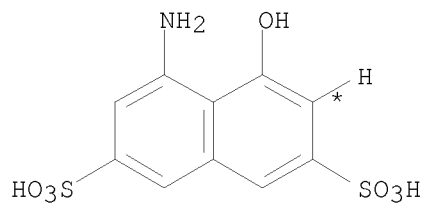
AQ



AR



AT

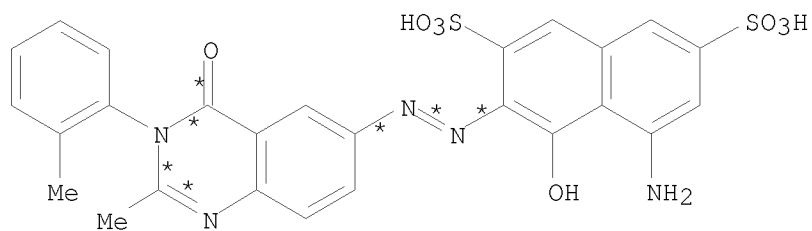


B

5  
STEPS  
→



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● 2 Na

C  
YIELD 86%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(1) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

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SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT B 90-20-0

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

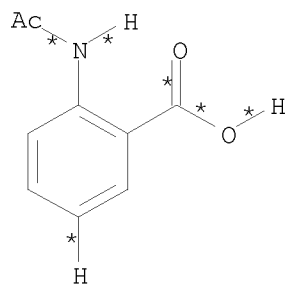
STAGE(7)

SOL 68-12-2 DMF

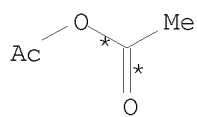
PRO C 313697-89-1

RX(80) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(2)

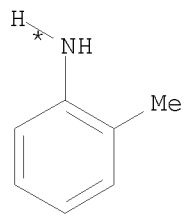
RX(80) AQ + AR + AT + K ==> L



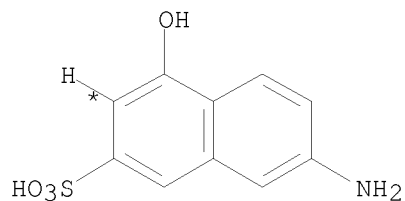
AQ



AR



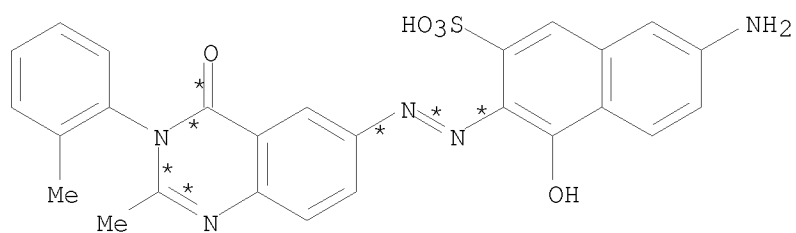
AT



K

5  
STEPS  
→

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● Na

L  
YIELD 79%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na<sub>2</sub>S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(2) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

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SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT K 87-02-5

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

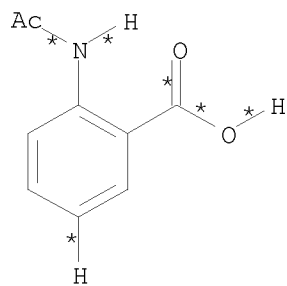
STAGE(7)

SOL 68-12-2 DMF

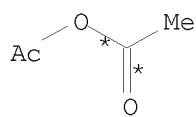
PRO L 313697-90-4

RX(81) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(3)

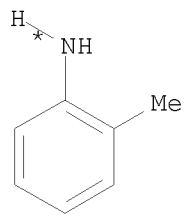
RX(81) AQ + AR + AT + M ==> N



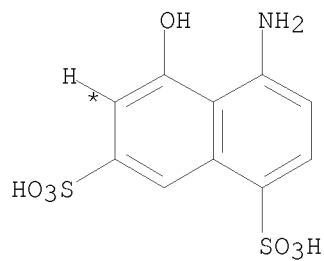
AQ



AR



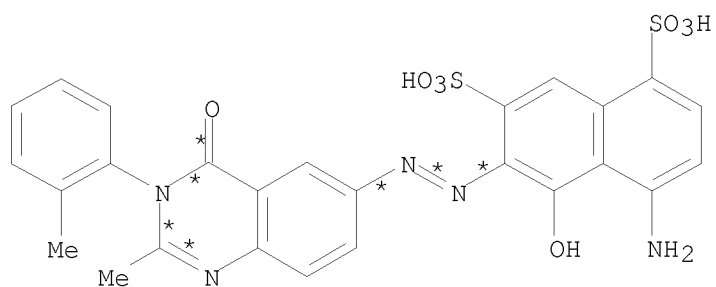
AT



M

5  
STEPS  
→

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● 2 Na

N  
YIELD 75%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na<sub>2</sub>S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(3) RCT A 963-34-8

STAGE(1)

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RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2  
SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT M 130-23-4  
SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

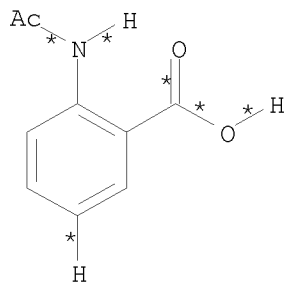
RGT H 7647-14-5 NaCl

STAGE(7)

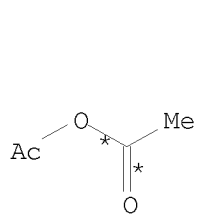
SOL 68-12-2 DMF

PRO N 313697-91-5

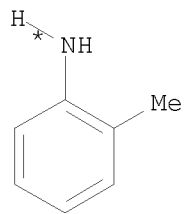
RX(82) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(4)  
RX(82) AQ + AR + AT + O ==> P



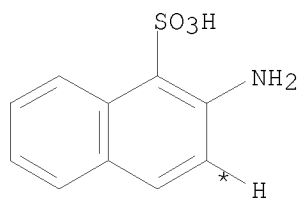
AQ



AR



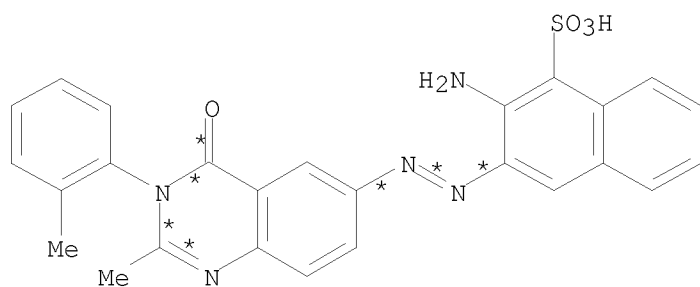
AT



O

5  
STEPS  
→

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● Na

P  
YIELD 82%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(4) RCT A 963-34-8

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STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT O 81-16-3

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

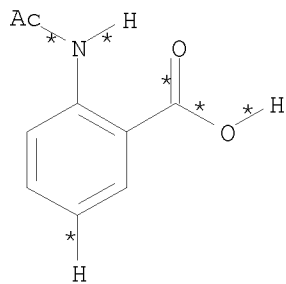
STAGE(7)

SOL 68-12-2 DMF

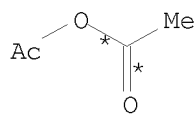
PRO P 313697-92-6

RX(83) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(5)

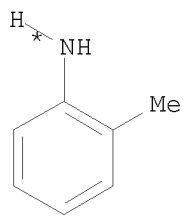
RX(83) AQ + AR + AT + Q ==> R



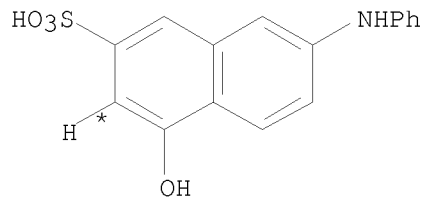
AQ



AR



AT

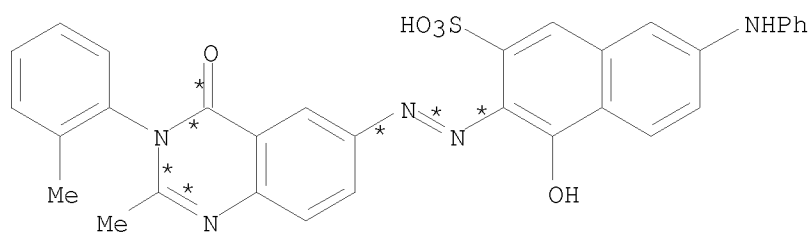


Q

5  
STEPS  
→



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● Na

R  
YIELD 84%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na<sub>2</sub>S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(5) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

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STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT Q 119-40-4

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

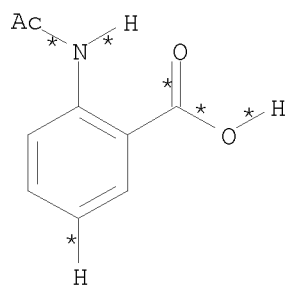
STAGE(7)

SOL 68-12-2 DMF

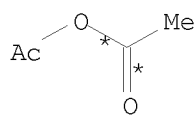
PRO R 313697-93-7

RX(84) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(6)

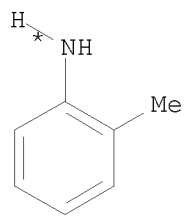
RX(84) AQ + AR + AT + S ==> T



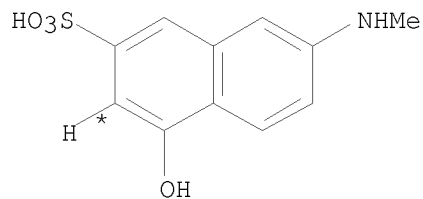
AQ



AR



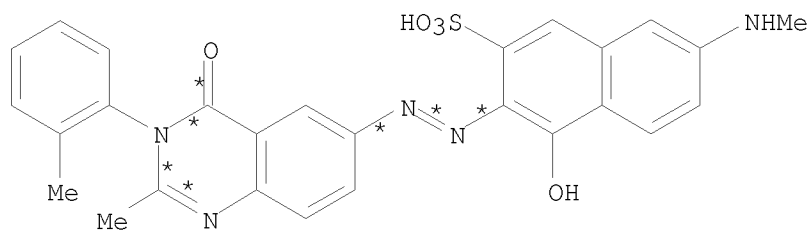
AT



S

5  
STEPS  
→

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● Na

T  
YIELD 76%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(6) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

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SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT S 22346-43-6

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

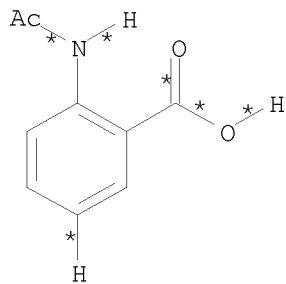
STAGE(7)

SOL 68-12-2 DMF

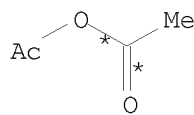
PRO T 313697-94-8

RX(85) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(7)

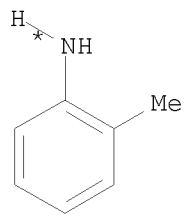
RX(85) AQ + AR + AT + U ==> V



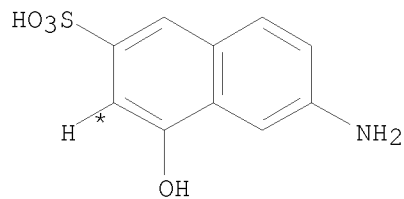
AQ



AR



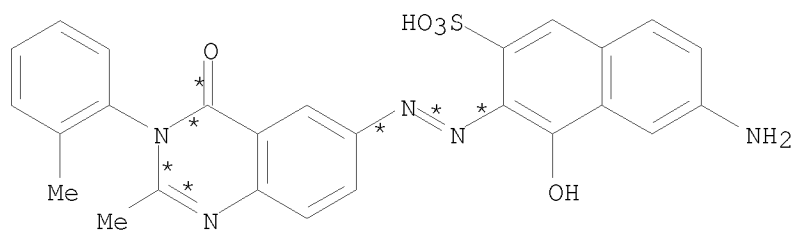
AT



U

5  
STEPS  
→

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● Na

V  
YIELD 87%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(7) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

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SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT U 90-51-7

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

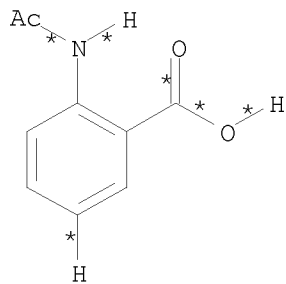
STAGE(7)

SOL 68-12-2 DMF

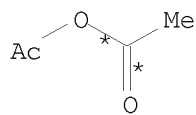
PRO V 313697-95-9

RX(86) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(8)

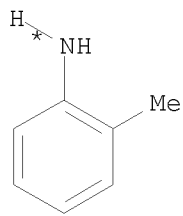
RX(86) AQ + AR + AT + W ==> X



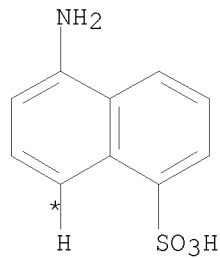
AQ



AR



AT



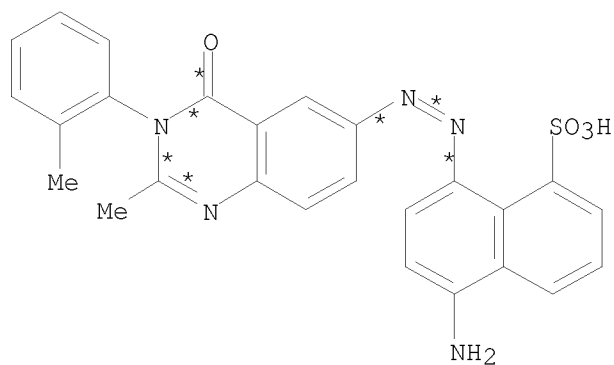
W

5

STEPS



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● Na

X  
YIELD 78%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na<sub>2</sub>S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

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RX(8) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT W 84-89-9

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

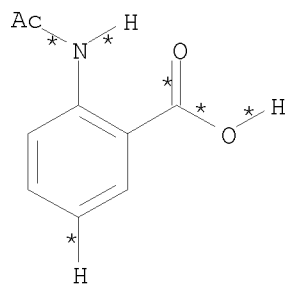
STAGE(7)

SOL 68-12-2 DMF

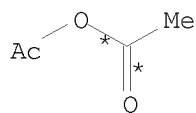
PRO X 313697-96-0

RX(87) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(9)

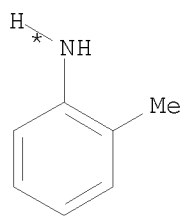
RX(87) AQ + AR + AT + Y ==> Z



AQ



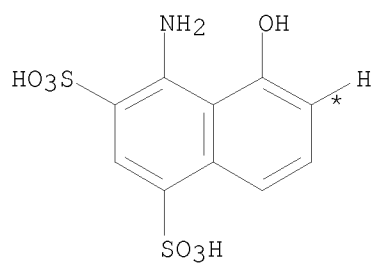
AR



AT

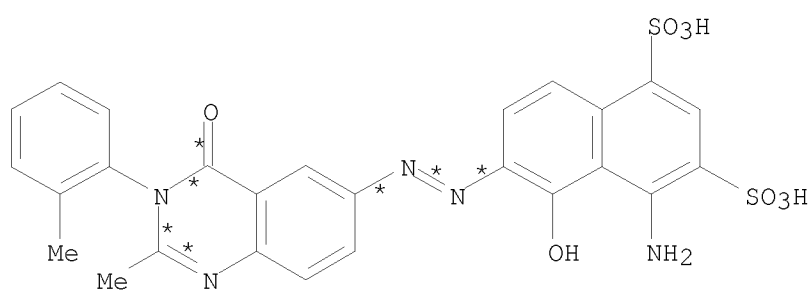


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Y

5  
STEPS  
→



● 2 Na

Z  
YIELD 88%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

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RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(9) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT Y 82-47-3

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

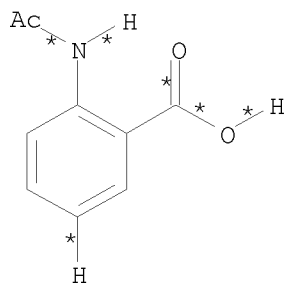
STAGE(7)

SOL 68-12-2 DMF

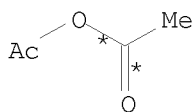
PRO Z 313697-97-1

RX(88) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(10)

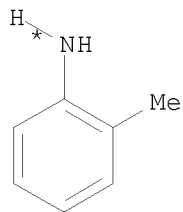
RX(88) AQ + AR + AT + AA ==> AB



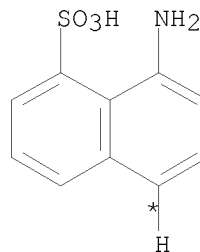
AQ



AR



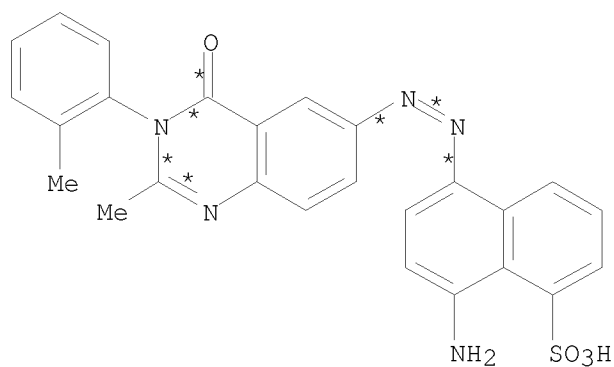
AT



AA

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5  
STEPS  
→



● Na

AB  
YIELD 77%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na<sub>2</sub>S

SOL 7732-18-5 Water

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STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(10) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT AA 82-75-7

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

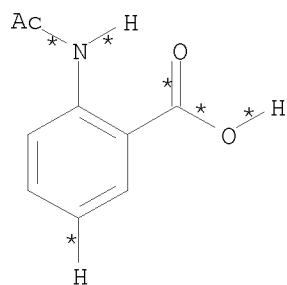
STAGE(7)

SOL 68-12-2 DMF

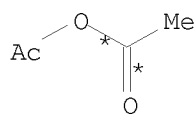
PRO AB 313697-98-2

RX(89) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(11)

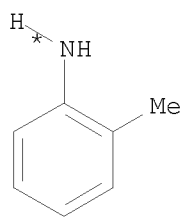
RX(89) AQ + AR + AT + AC ==> AD



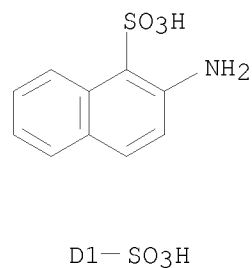
AQ



AR



AT



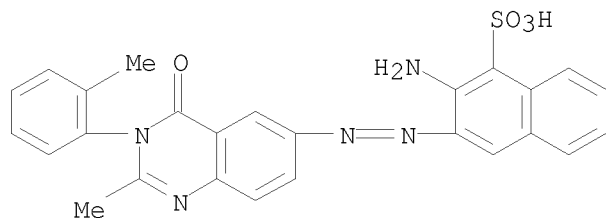
AC

5

STEPS



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D1-SO<sub>3</sub>H

●2 Na

AD  
YIELD 72%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na<sub>2</sub>S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(11) RCT A 963-34-8

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STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT AC 171570-11-9

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

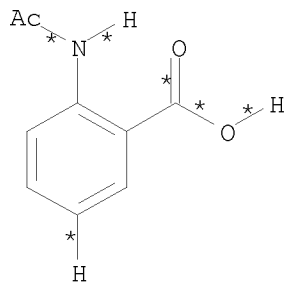
STAGE(7)

SOL 68-12-2 DMF

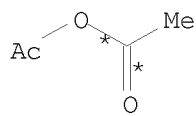
PRO AD 314730-80-8

RX(90) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(12)

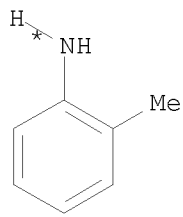
RX(90) AQ + AR + AT + AE ==> AF



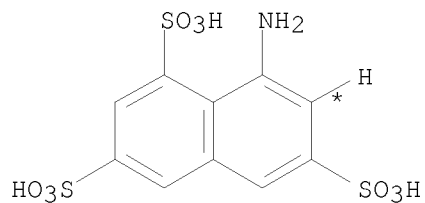
AQ



AR



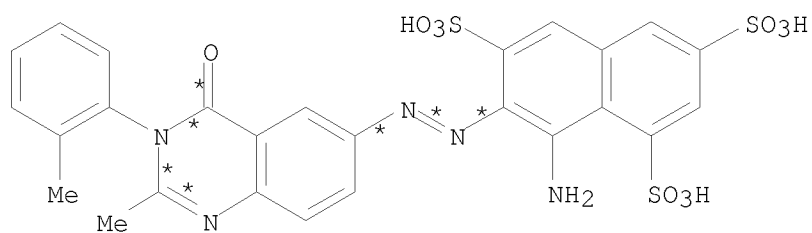
AT



AE

5  
STEPS  
→

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● 3 Na

AF  
YIELD 78%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(12) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

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SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT AE 117-42-0

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

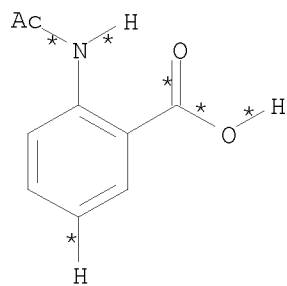
STAGE(7)

SOL 68-12-2 DMF

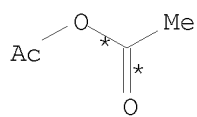
PRO AF 313697-99-3

RX(91) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(13)

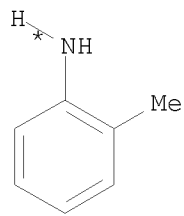
RX(91) AQ + AR + AT + AG ==> AH



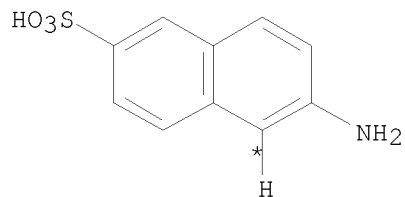
AQ



AR



AT

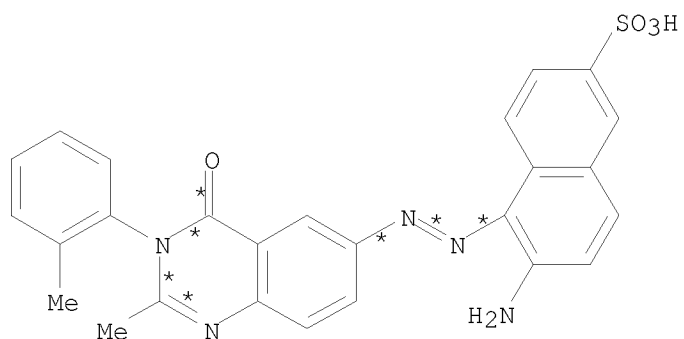


AG

5  
STEPS  
→



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● Na

AH

YIELD 83%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na<sub>2</sub>S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

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RX(13) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT AG 93-00-5

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

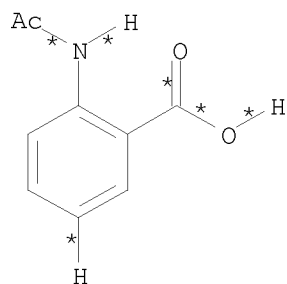
STAGE(7)

SOL 68-12-2 DMF

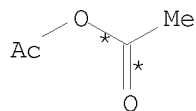
PRO AH 313698-00-9

RX(92) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(14)

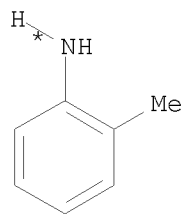
RX(92) AQ + AR + AT + AI ==> AJ



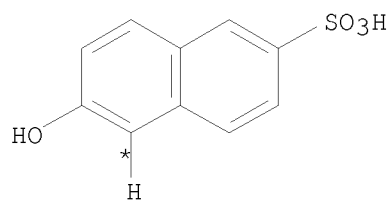
AQ



AR



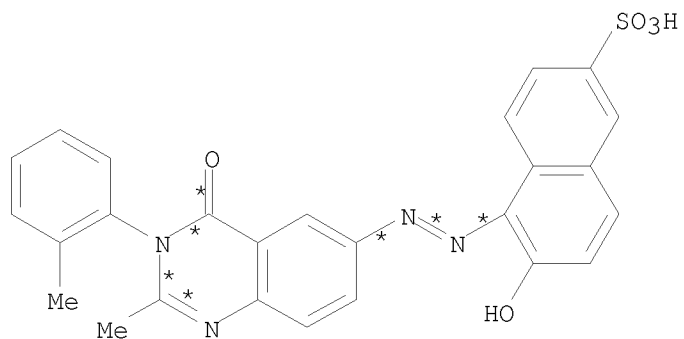
AT



AI

5  
STEPS  
→

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● Na

AJ

YIELD 86%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na<sub>2</sub>S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

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RX(14) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT AI 93-01-6

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

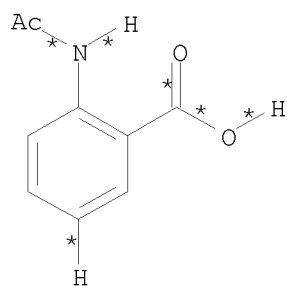
STAGE(7)

SOL 68-12-2 DMF

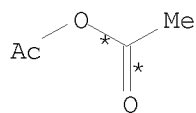
PRO AJ 313698-01-0

RX(93) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(15)

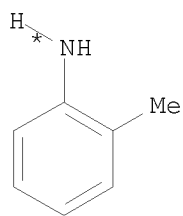
RX(93) AQ + AR + AT + AK ==> AL



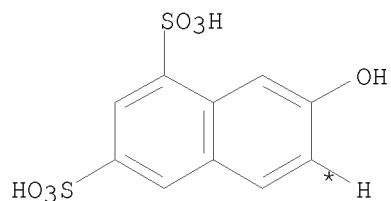
AQ



AR



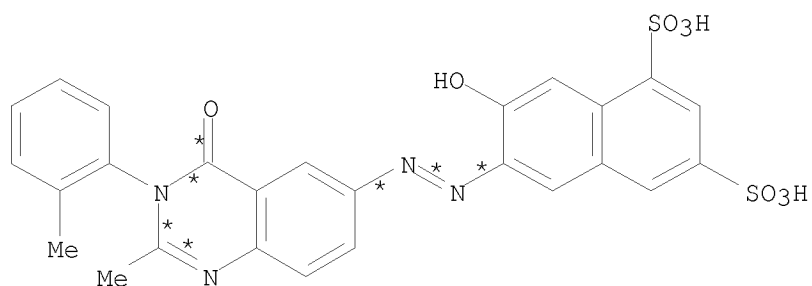
AT



AK

5  
STEPS  
→

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● 2 Na

AL

YIELD 82%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na<sub>2</sub>S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

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RX(15) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT AK 118-32-1

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

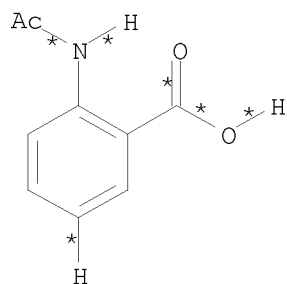
STAGE(7)

SOL 68-12-2 DMF

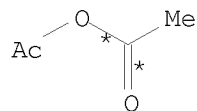
PRO AL 313698-02-1

RX(94) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(16)

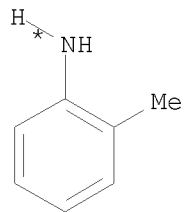
RX(94) AQ + AR + AT + AM ==> AN



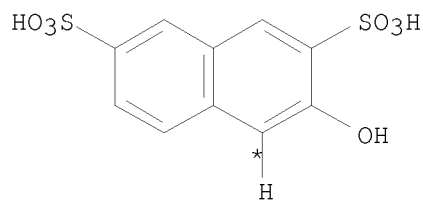
AQ



AR



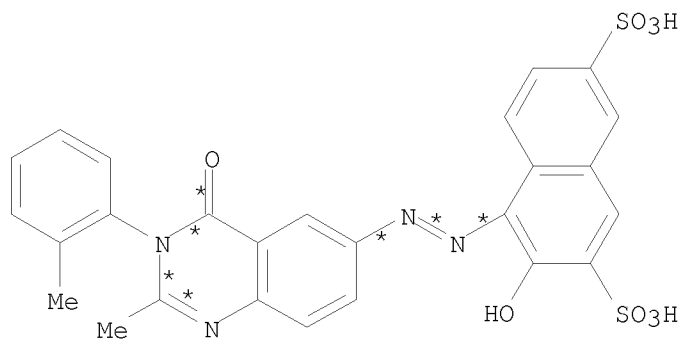
AT



AM

5  
STEPS  
→

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● 2 Na

AN

YIELD 75%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na<sub>2</sub>S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

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RX(16) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT AM 148-75-4

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

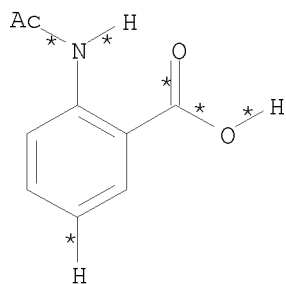
STAGE(7)

SOL 68-12-2 DMF

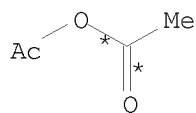
PRO AN 313698-03-2

RX(95) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(17)

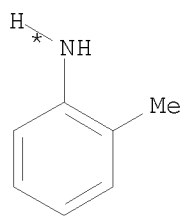
RX(95) AQ + AR + AT + AO ==> AP



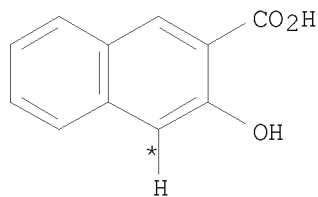
AQ



AR



AT

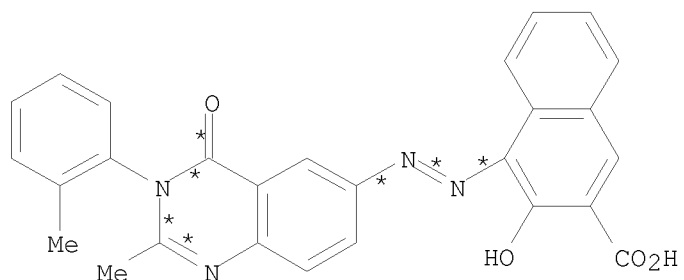


AO

5  
STEPS  
→



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● Na

AP  
YIELD 81%

RX(18) RCT AQ 89-52-1, AR 108-24-7  
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na<sub>2</sub>S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

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RX(17) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl  
SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2  
SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT AO 92-70-6  
SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

STAGE(7)

SOL 68-12-2 DMF

PRO AP 313698-04-3

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 113 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 134:72894 CASREACT

TITLE: Quinazoline dyes: synthesis of  
2-styryl-6-arylazo-4-oxoquinazoline dyes and their  
application on silk, wool and viscose rayon

AUTHOR(S): Patel, K. C.; Patel, S. K.; Desai, K. R.

CORPORATE SOURCE: Department of Chemistry, South Gujarat University,  
Surat, 395007, India

SOURCE: Acta Ciencia Indica, Chemistry (1999), 25(3), 41-48  
CODEN: ACICDV; ISSN: 0253-7338

PUBLISHER: Pragati Prakashan

DOCUMENT TYPE: Journal

LANGUAGE: English

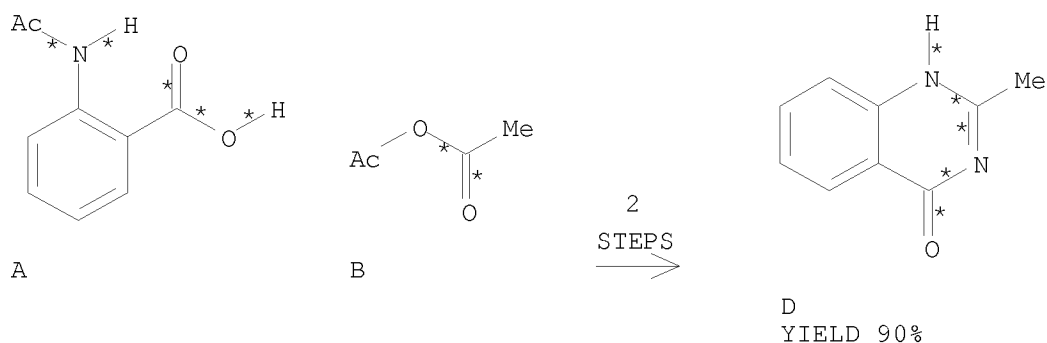
AB Various quinazoline dyes have been prepared by coupling of diazotized  
2-styryl-6-amino-4-oxoquinazoline with various coupling components such as  
H-acid, J-acid, N-methyl-J-acid, N-phenyl-J-acid, Gamma acid, G-acid,  
R-salt, Schaffer's acid, 1-phenyl-3-methyl-5-pyrazolone,  
1-(4'-sulfophenyl)-3-methyl-5-pyrazolone, 1-(2',5'-  
dichloro-4'-sulfophenyl)-3-methyl-5-pyrazolone,  
1-(4'-sulfophenyl)-3-carboxy-5-pyrazolone and peri acid and their dyeing  
performance of direct dyes has been assessed on viscose rayon and as acid  
dyes has been assessed on silk and wool fibers. The purity of all dyes  
have been checked by thin-layer chromatog. The value of percentage found  
of N of all these dyes is in good agreement with the calculated values. The  
IR spectra of all these dyes showed all characteristic band present in the  
dye mols. The % exhaustion of dye-bath on silk and wool was good to

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excellent and on viscose rayon it was poor to moderate. A study of the fastness of dyed patterns showed that the dyes were good to very good for silk and wool, and fair to good for viscose rayon.

RX(19) OF 93 COMPOSED OF RX(1), RX(2)

RX(19) A + B ==> D



RX(1) RCT A 89-52-1, B 108-24-7

PRO C 525-76-8

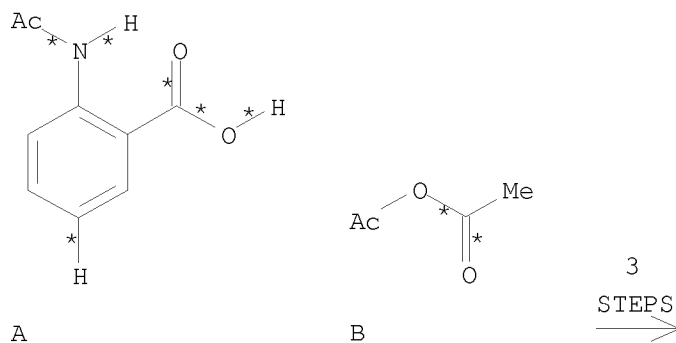
RX(2) RCT C 525-76-8

RGT E 7664-41-7 NH3

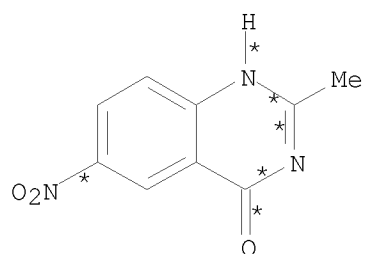
PRO D 1769-24-0

RX(36) OF 93 COMPOSED OF RX(1), RX(2), RX(3)

RX(36) A + B ==> F



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F  
YIELD 95%

RX(1) RCT A 89-52-1, B 108-24-7  
PRO C 525-76-8

RX(2) RCT C 525-76-8  
RGT E 7664-41-7 NH3  
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

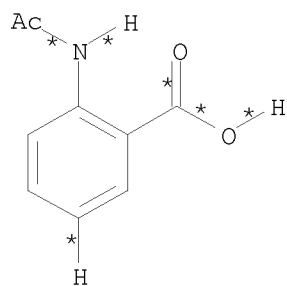
STAGE(2)

SOL 7732-18-5 Water

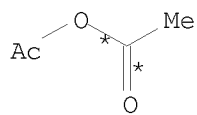
PRO F 24688-36-6

RX(38) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4)

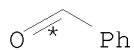
RX(38) A + B + J ==> K



A



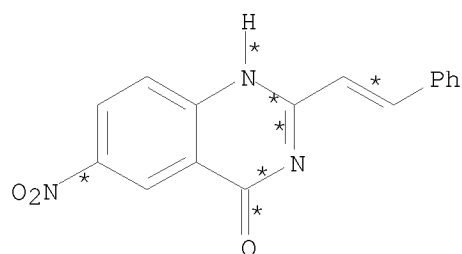
B



J

4  
STEPS  
→

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K  
YIELD 80%

RX(1) RCT A 89-52-1, B 108-24-7  
PRO C 525-76-8

RX(2) RCT C 525-76-8  
RGT E 7664-41-7 NH3  
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

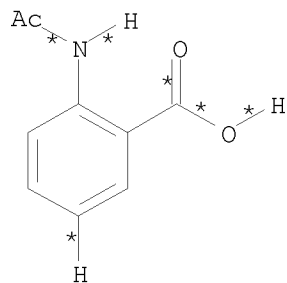
STAGE(2)

RCT J 100-52-7

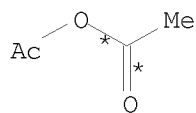
PRO K 24688-33-3

RX(67) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5)

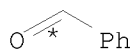
RX(67) A + B + J ==> L



A



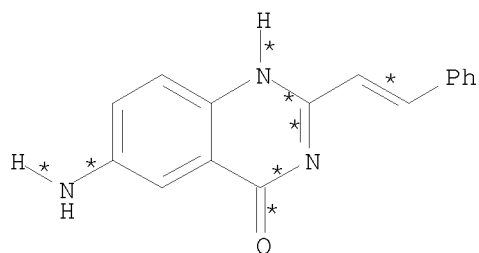
B



J

5  
STEPS  
→

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L  
YIELD 88%

RX(1) RCT A 89-52-1, B 108-24-7  
PRO C 525-76-8

RX(2) RCT C 525-76-8  
RGT E 7664-41-7 NH3  
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

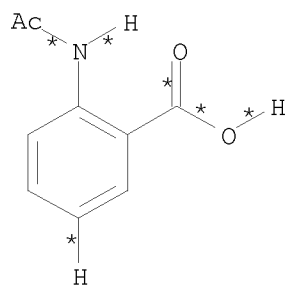
STAGE(2)

RCT J 100-52-7

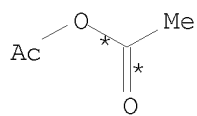
PRO K 24688-33-3

RX(5) RCT K 24688-33-3  
RGT M 1313-82-2 Na2S  
PRO L 30896-48-1  
SOL 7732-18-5 Water

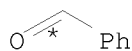
RX(81) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6)  
RX(81) A + B + J + N ==> O



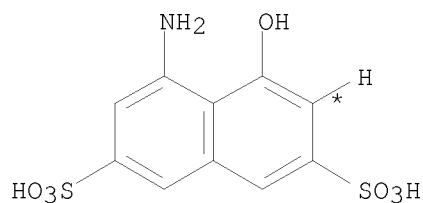
A



B

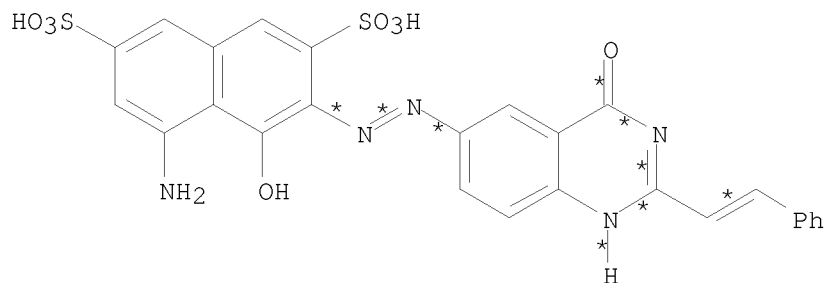


J



N

6  
STEPS  
→



O  
YIELD 84%

RX(1) RCT A 89-52-1, B 108-24-7  
PRO C 525-76-8

RX(2) RCT C 525-76-8  
RGT E 7664-41-7 NH3  
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

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PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3

RGT M 1313-82-2 Na2S

PRO L 30896-48-1

SOL 7732-18-5 Water

RX(6) RCT L 30896-48-1

STAGE(1)

RGT P 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT Q 7632-00-0 NaNO2

STAGE(3)

RGT G 7664-93-9 H2SO4

STAGE(4)

RCT N 90-20-0

RGT R 144-55-8 NaHCO3

SOL 7732-18-5 Water

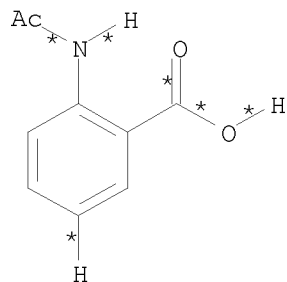
STAGE(5)

RGT S 7647-14-5 NaCl

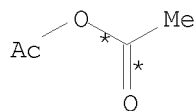
PRO O 315681-02-8

RX(82) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(7)

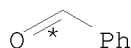
RX(82) A + B + J + T ==> U



A



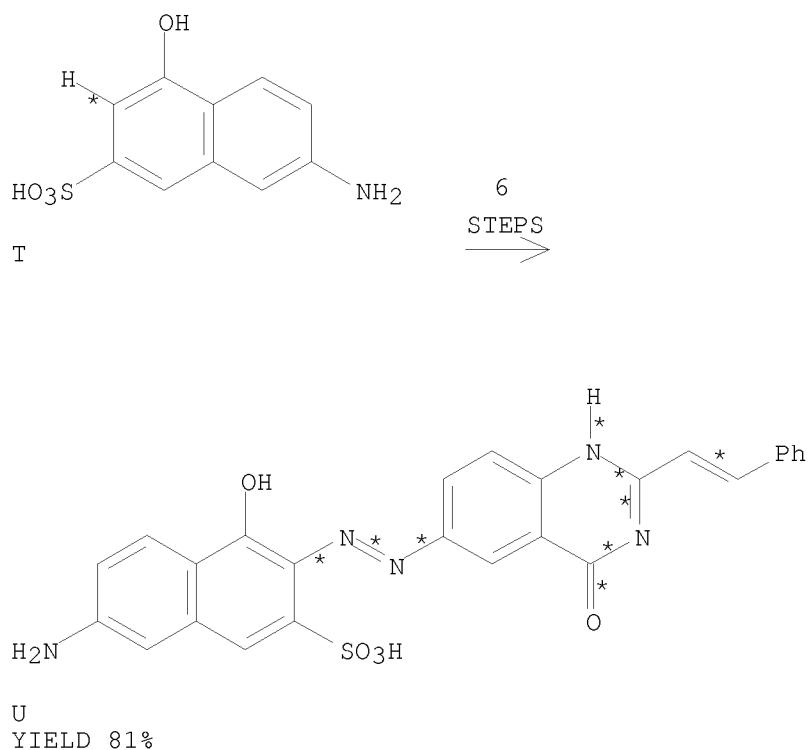
B



J



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RX(1) RCT A 89-52-1, B 108-24-7  
PRO C 525-76-8

RX(2) RCT C 525-76-8  
RGT E 7664-41-7 NH<sub>3</sub>  
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, H 7697-37-2 HNO<sub>3</sub>

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac<sub>2</sub>O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3  
RGT M 1313-82-2 Na<sub>2</sub>S  
PRO L 30896-48-1  
SOL 7732-18-5 Water

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RX(7) RCT L 30896-48-1

STAGE(1)

RGT P 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT Q 7632-00-0 NaNO2

STAGE(3)

RGT G 7664-93-9 H2SO4

STAGE(4)

RCT T 87-02-5

RGT R 144-55-8 NaHCO3

SOL 7732-18-5 Water

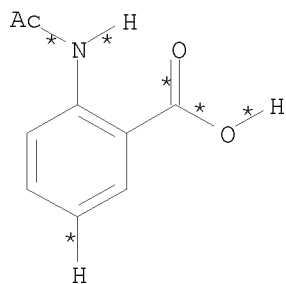
STAGE(5)

RGT S 7647-14-5 NaCl

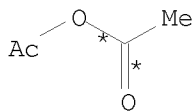
PRO U 315681-03-9

RX(83) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(8)

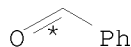
RX(83) A + B + J + V ==> W



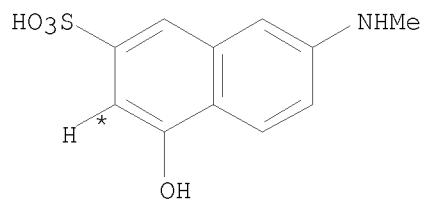
A



B



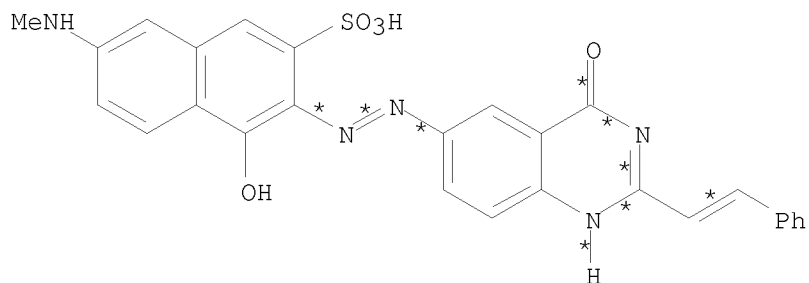
J



V

6  
STEPS  
→

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W  
YIELD 82%

RX(1) RCT A 89-52-1, B 108-24-7  
PRO C 525-76-8

RX(2) RCT C 525-76-8  
RGT E 7664-41-7 NH<sub>3</sub>  
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, H 7697-37-2 HNO<sub>3</sub>

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac<sub>2</sub>O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3  
RGT M 1313-82-2 Na<sub>2</sub>S  
PRO L 30896-48-1  
SOL 7732-18-5 Water

RX(8) RCT L 30896-48-1

STAGE(1)

RGT P 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT Q 7632-00-0 NaNO<sub>2</sub>

STAGE(3)

RGT G 7664-93-9 H<sub>2</sub>SO<sub>4</sub>

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STAGE(4)

RCT V 22346-43-6

RGT R 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water

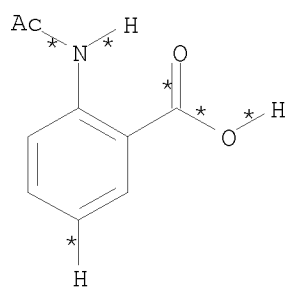
STAGE(5)

RGT S 7647-14-5 NaCl

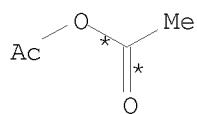
PRO W 315681-04-0

RX(84) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(9)

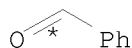
RX(84) A + B + J + X ==> Y



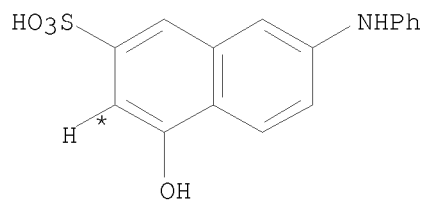
A



B

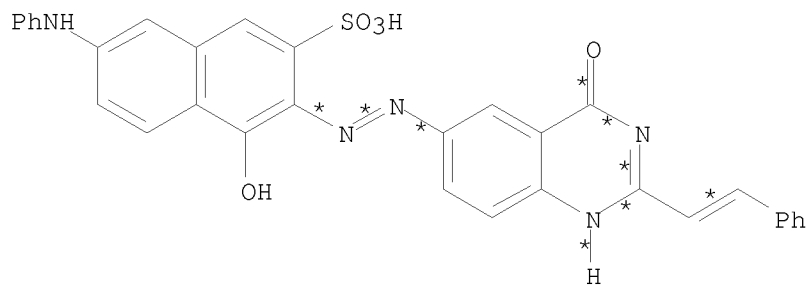


J



X

6  
STEPS  
→



Y

YIELD 86%

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RX(1) RCT A 89-52-1, B 108-24-7  
PRO C 525-76-8

RX(2) RCT C 525-76-8  
RGT E 7664-41-7 NH3  
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3  
RGT M 1313-82-2 Na2S  
PRO L 30896-48-1  
SOL 7732-18-5 Water

RX(9) RCT L 30896-48-1

STAGE(1)

RGT P 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT Q 7632-00-0 NaNO2

STAGE(3)

RGT G 7664-93-9 H2SO4

STAGE(4)

RCT X 119-40-4

RGT R 144-55-8 NaHCO3

SOL 7732-18-5 Water

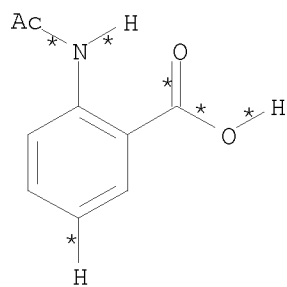
STAGE(5)

RGT S 7647-14-5 NaCl

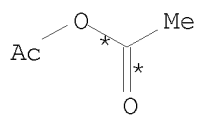
PRO Y 315681-05-1

RX(85) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(10)

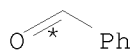
RX(85) A + B + J + Z ==> AA



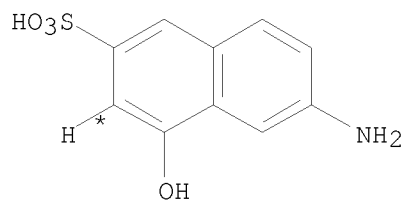
A



B

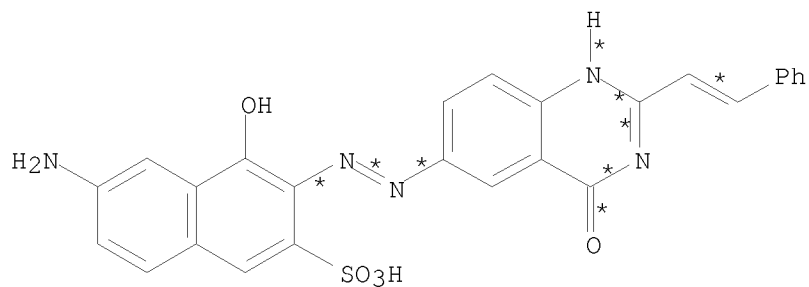


J



Z

6  
STEPS  
→



AA  
YIELD 81%

RX(1) RCT A 89-52-1, B 108-24-7  
PRO C 525-76-8

RX(2) RCT C 525-76-8  
RGT E 7664-41-7 NH3  
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

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PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)  
RGT B 108-24-7 Ac2O

STAGE(2)  
RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3  
RGT M 1313-82-2 Na2S  
PRO L 30896-48-1  
SOL 7732-18-5 Water

RX(10) RCT L 30896-48-1

STAGE(1)  
RGT P 7647-01-0 HCl  
SOL 7732-18-5 Water

STAGE(2)  
RGT Q 7632-00-0 NaNO2

STAGE(3)  
RGT G 7664-93-9 H2SO4

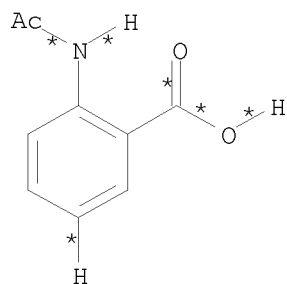
STAGE(4)  
RCT Z 90-51-7  
RGT R 144-55-8 NaHCO3  
SOL 7732-18-5 Water

STAGE(5)  
RGT S 7647-14-5 NaCl

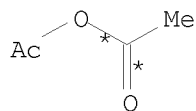
PRO AA 315681-06-2

RX(86) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(11)

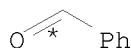
RX(86) A + B + J + AB ==> AC



A

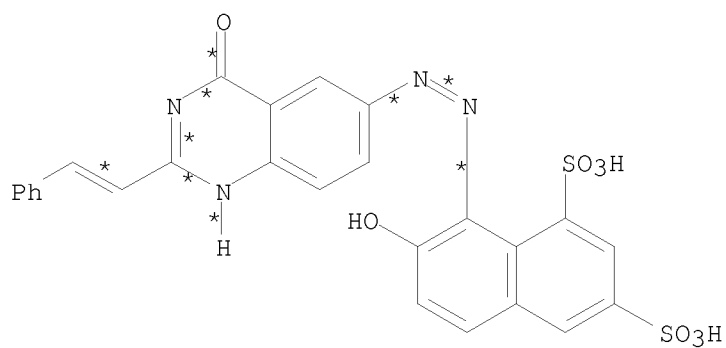
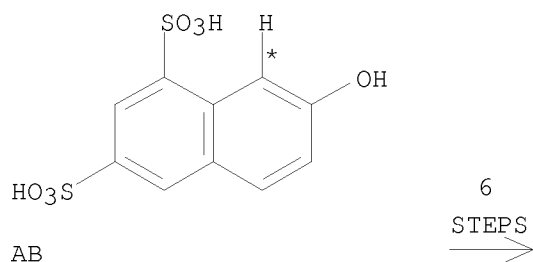


B



J

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AC  
YIELD 80%

RX(1) RCT A 89-52-1, B 108-24-7  
PRO C 525-76-8

RX(2) RCT C 525-76-8  
RGT E 7664-41-7 NH3  
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3  
RGT M 1313-82-2 Na2S



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PRO L 30896-48-1  
SOL 7732-18-5 Water

RX(11) RCT L 30896-48-1

STAGE(1)  
RGT P 7647-01-0 HCl  
SOL 7732-18-5 Water

STAGE(2)  
RGT Q 7632-00-0 NaNO2

STAGE(3)  
RGT G 7664-93-9 H2SO4

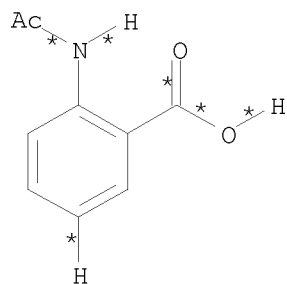
STAGE(4)  
RCT AB 118-32-1  
RGT R 144-55-8 NaHCO3  
SOL 7732-18-5 Water

STAGE(5)  
RGT S 7647-14-5 NaCl

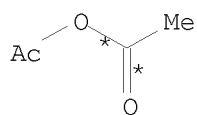
PRO AC 315681-07-3

RX(87) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(12)

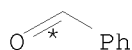
RX(87) A + B + J + AD ==> AE



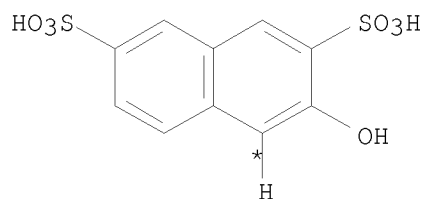
A



B



J

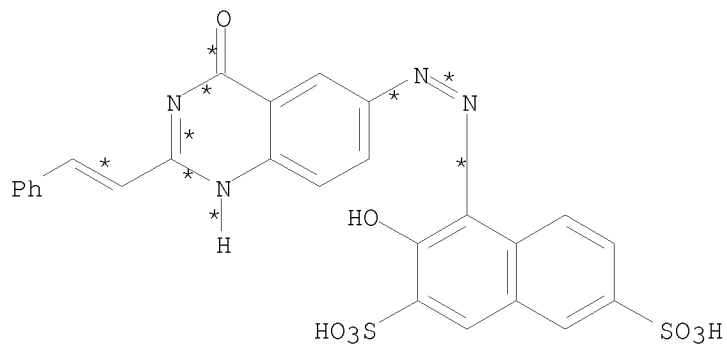


● 2 Na

6  
STEPS  
→

AD

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● 2 Na

AE  
YIELD 84%

RX(1) RCT A 89-52-1, B 108-24-7  
PRO C 525-76-8

RX(2) RCT C 525-76-8  
RGT E 7664-41-7 NH<sub>3</sub>  
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)  
RGT G 7664-93-9 H<sub>2</sub>SO<sub>4</sub>, H 7697-37-2 HNO<sub>3</sub>

STAGE(2)  
SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)  
RGT B 108-24-7 Ac<sub>2</sub>O

STAGE(2)  
RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3  
RGT M 1313-82-2 Na<sub>2</sub>S  
PRO L 30896-48-1  
SOL 7732-18-5 Water

RX(12) RCT L 30896-48-1

STAGE(1)  
RGT P 7647-01-0 HCl

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SOL 7732-18-5 Water

STAGE(2)

RGT Q 7632-00-0 NaNO2

STAGE(3)

RGT G 7664-93-9 H2SO4

STAGE(4)

RCT AD 135-51-3

RGT R 144-55-8 NaHCO3

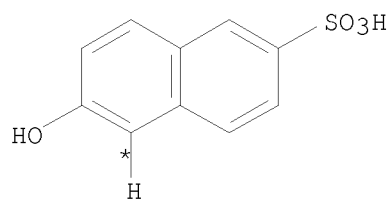
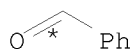
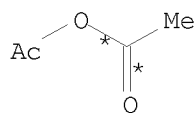
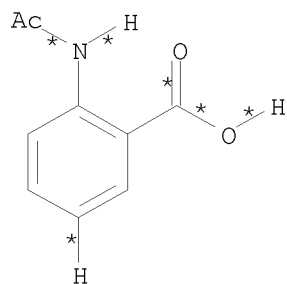
SOL 7732-18-5 Water

STAGE(5)

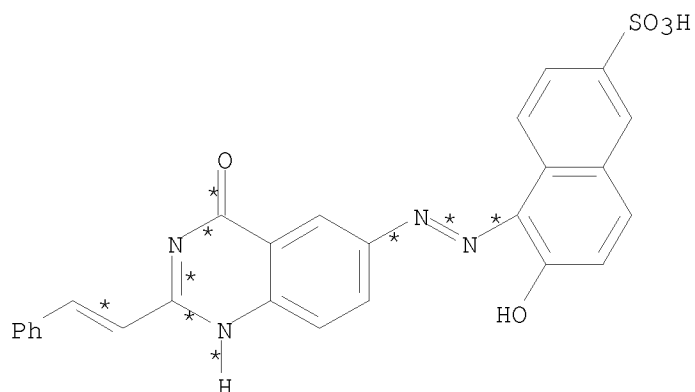
RGT S 7647-14-5 NaCl

PRO AE 315681-08-4

RX(88) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(13)  
RX(88) A + B + J + AF ==> AG



6  
STEPS  
→



AG

YIELD 79%

RX(1) RCT A 89-52-1, B 108-24-7  
PRO C 525-76-8

RX(2) RCT C 525-76-8  
RGT E 7664-41-7 NH3  
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3  
RGT M 1313-82-2 Na2S  
PRO L 30896-48-1  
SOL 7732-18-5 Water

RX(13) RCT L 30896-48-1

STAGE(1)

RGT P 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

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RGT Q 7632-00-0 NaNO2

STAGE(3)

RGT G 7664-93-9 H2SO4

STAGE(4)

RCT AF 93-01-6

RGT R 144-55-8 NaHCO3

SOL 7732-18-5 Water

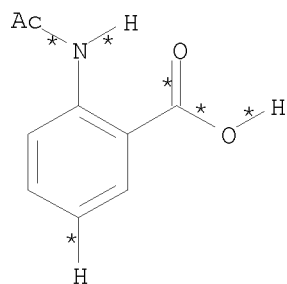
STAGE(5)

RGT S 7647-14-5 NaCl

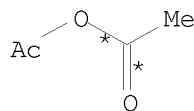
PRO AG 315681-09-5

RX(89) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(14)

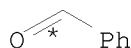
RX(89) A + B + J + AH ==> AI



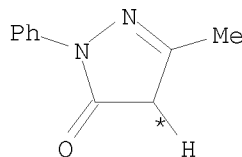
A



B

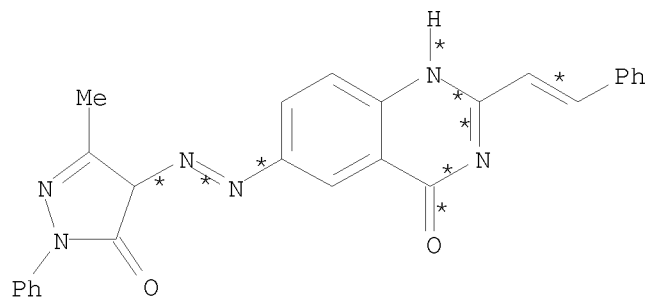


J



AH

6  
STEPS  
→



AI  
YIELD 86%

RX(1) RCT A 89-52-1, B 108-24-7  
PRO C 525-76-8

RX(2) RCT C 525-76-8  
RGT E 7664-41-7 NH3  
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

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```

      STAGE(1)
      RGT  G 7664-93-9 H2SO4, H 7697-37-2 HNO3

      STAGE(2)
      SOL  7732-18-5 Water

PRO   F 24688-36-6

RX(4)  RCT  F 24688-36-6

      STAGE(1)
      RGT  B 108-24-7 Ac2O

      STAGE(2)
      RCT  J 100-52-7

PRO   K 24688-33-3

RX(5)  RCT  K 24688-33-3
      RGT  M 1313-82-2 Na2S
      PRO  L 30896-48-1
      SOL  7732-18-5 Water

RX(14) RCT  L 30896-48-1

      STAGE(1)
      RGT  P 7647-01-0 HCl
      SOL  7732-18-5 Water

      STAGE(2)
      RGT  Q 7632-00-0 NaNO2

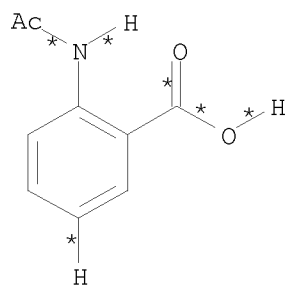
      STAGE(3)
      RGT  G 7664-93-9 H2SO4

      STAGE(4)
      RCT  AH 89-25-8
      RGT  R 144-55-8 NaHCO3
      SOL  7732-18-5 Water

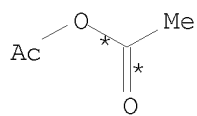
      STAGE(5)
      RGT  S 7647-14-5 NaCl

PRO   AI 315681-10-8

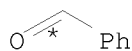

RX(90) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(15)
RX(90)   A  +  B  +  J  +  AJ  ==>  AK
```



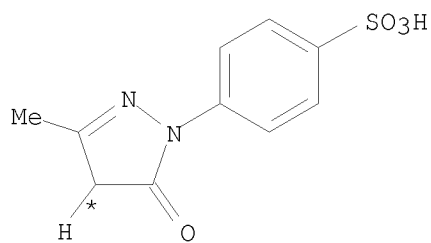
A



B

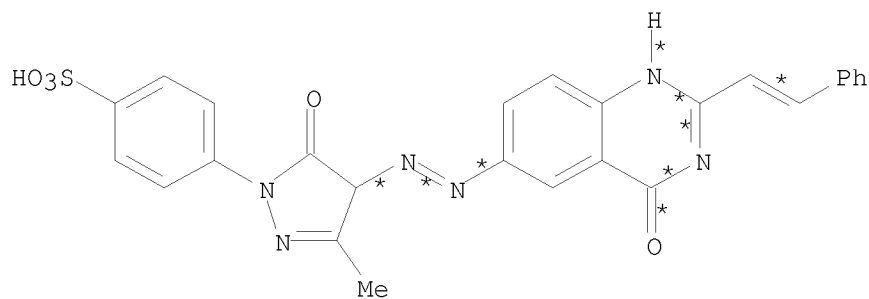


J



AJ

6  
STEPS  
→



AK  
YIELD 81%

RX(1) RCT A 89-52-1, B 108-24-7  
PRO C 525-76-8

RX(2) RCT C 525-76-8  
RGT E 7664-41-7 NH3  
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

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SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)  
RGT B 108-24-7 Ac2O

STAGE(2)  
RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3  
RGT M 1313-82-2 Na2S  
PRO L 30896-48-1  
SOL 7732-18-5 Water

RX(15) RCT L 30896-48-1

STAGE(1)  
RGT P 7647-01-0 HCl  
SOL 7732-18-5 Water

STAGE(2)  
RGT Q 7632-00-0 NaNO2

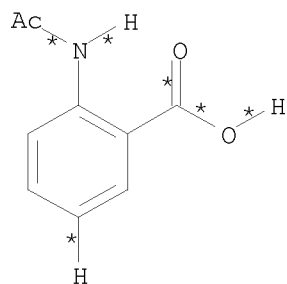
STAGE(3)  
RGT G 7664-93-9 H2SO4

STAGE(4)  
RCT AJ 89-36-1  
RGT R 144-55-8 NaHCO3  
SOL 7732-18-5 Water

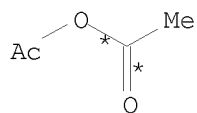
STAGE(5)  
RGT S 7647-14-5 NaCl

PRO AK 315681-11-9

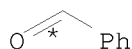
RX(91) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(16)  
RX(91) A + B + J + AL ==> AM



A



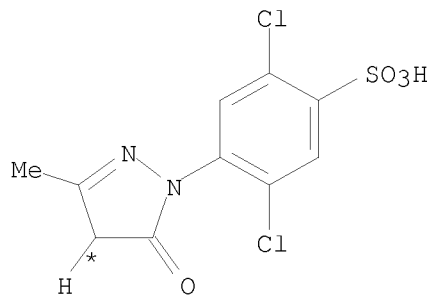
B



J

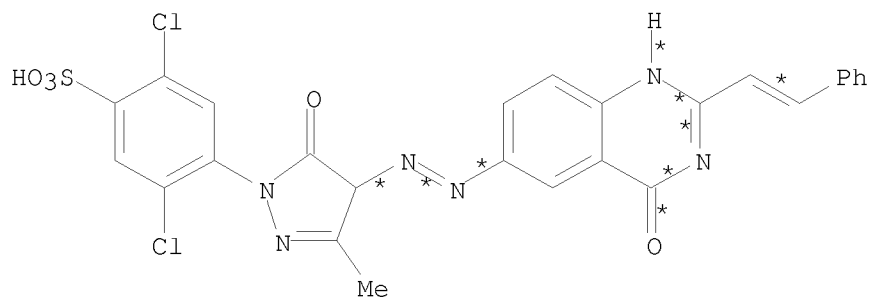


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AL

6  
STEPS  
→



AM

YIELD 78%

RX(1) RCT A 89-52-1, B 108-24-7  
PRO C 525-76-8

RX(2) RCT C 525-76-8  
RGT E 7664-41-7 NH3  
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

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RX(5)        RCT   K 24688-33-3  
              RGT   M 1313-82-2 Na2S  
              PRO   L 30896-48-1  
              SOL   7732-18-5 Water

RX(16)      RCT   L 30896-48-1

STAGE(1)

              RGT   P 7647-01-0 HCl  
              SOL   7732-18-5 Water

STAGE(2)

              RGT   Q 7632-00-0 NaNO2

STAGE(3)

              RGT   G 7664-93-9 H2SO4

STAGE(4)

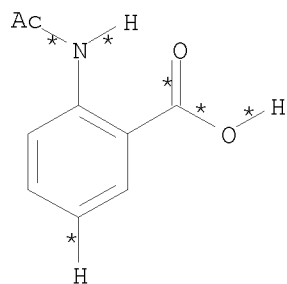
              RCT   AL 84-57-1  
              RGT   R 144-55-8 NaHCO3  
              SOL   7732-18-5 Water

STAGE(5)

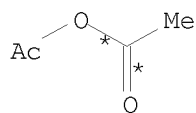
              RGT   S 7647-14-5 NaCl

PRO   AM 315681-12-0

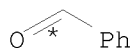
RX(92) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(17)  
RX(92)      A + B + J + AN ==> AO



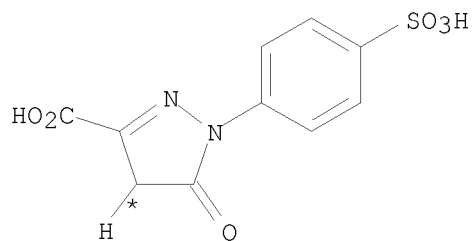
A



B



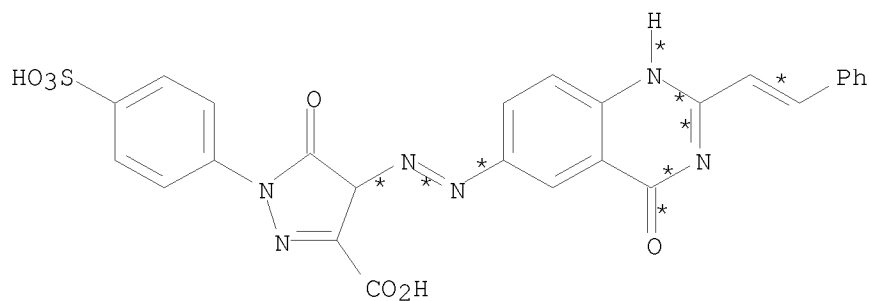
J



AN

6  
STEPS  
→

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AO  
YIELD 79%

RX(1) RCT A 89-52-1, B 108-24-7  
PRO C 525-76-8

RX(2) RCT C 525-76-8  
RGT E 7664-41-7 NH3  
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3  
RGT M 1313-82-2 Na2S  
PRO L 30896-48-1  
SOL 7732-18-5 Water

RX(17) RCT L 30896-48-1

STAGE(1)

RGT P 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT Q 7632-00-0 NaNO2

STAGE(3)

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RGT G 7664-93-9 H2SO4

STAGE(4)

RCT AN 118-47-8

RGT R 144-55-8 NaHCO3

SOL 7732-18-5 Water

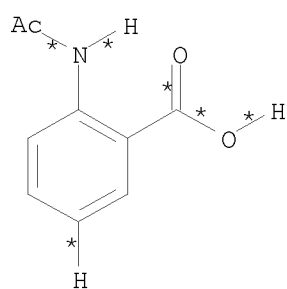
STAGE(5)

RGT S 7647-14-5 NaCl

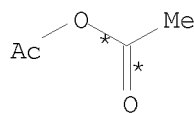
PRO AO 315681-13-1

RX(93) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(18)

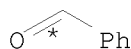
RX(93) A + B + J + AP ==> AQ



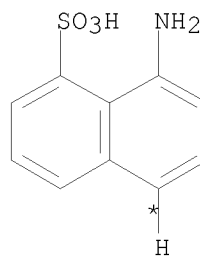
A



B

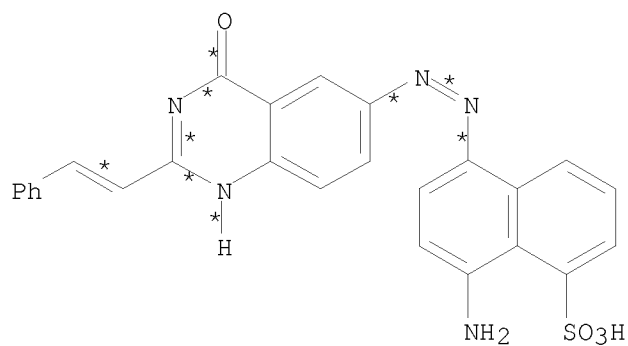


J



AP

6  
STEPS  
=>



AQ

YIELD 78%

RX(1) RCT A 89-52-1, B 108-24-7  
PRO C 525-76-8

RX(2) RCT C 525-76-8  
RGT E 7664-41-7 NH3  
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

## STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

## STAGE(1)

RGT B 108-24-7 Ac2O

## STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3

RGT M 1313-82-2 Na2S

PRO L 30896-48-1

SOL 7732-18-5 Water

RX(18) RCT L 30896-48-1

## STAGE(1)

RGT P 7647-01-0 HCl

SOL 7732-18-5 Water

## STAGE(2)

RGT Q 7632-00-0 NaNO2

## STAGE(3)

RGT G 7664-93-9 H2SO4

## STAGE(4)

RCT AP 82-75-7

RGT R 144-55-8 NaHCO3

SOL 7732-18-5 Water

## STAGE(5)

RGT S 7647-14-5 NaCl

PRO AQ 315681-14-2

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 114 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 134:4911 CASREACT  
TITLE: Synthesis of quinazoline compound  
AUTHOR(S): Shi, Qingqing; Liu, Zhiping  
CORPORATE SOURCE: Shanghai Research Institute of Chemical Reagent,  
Shanghai, 200333, Peop. Rep. China  
SOURCE: Shanghai Huagong (2000), 25(9), 18-20  
CODEN: SHAHE2; ISSN: 1004-017X  
PUBLISHER: Shanghai Huagong Bianjibu  
DOCUMENT TYPE: Journal

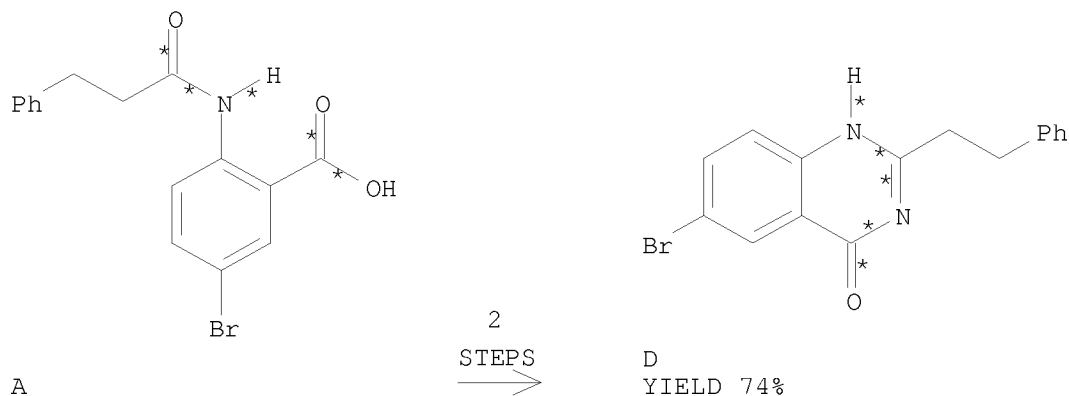
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LANGUAGE: Chinese

AB 6-Cyano-2-(2-phenylethyl)quinazolinone was prepared in 5 steps in 30.6% overall yield from 2-aminobenzoic acid.

RX(6) OF 15 COMPOSED OF RX(1), RX(2)

RX(6) A ==> D

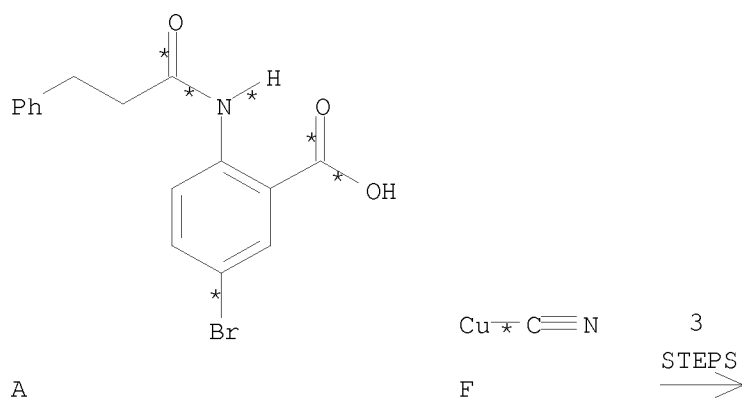


RX(1) RCT A 307001-06-5  
PRO B 307001-07-6  
SOL 108-24-7 Ac2O

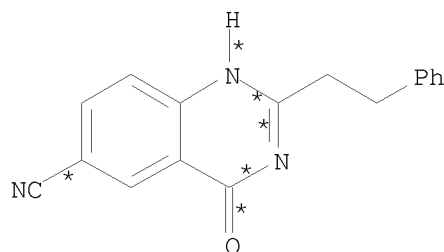
RX(2) RCT B 307001-07-6  
RGT E 75-12-7 Formamide  
PRO D 307001-08-7

RX(10) OF 15 COMPOSED OF RX(1), RX(2), RX(3)

RX(10) A + F ==> G



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G  
YIELD 78%

RX(1) RCT A 307001-06-5  
PRO B 307001-07-6  
SOL 108-24-7 Ac2O

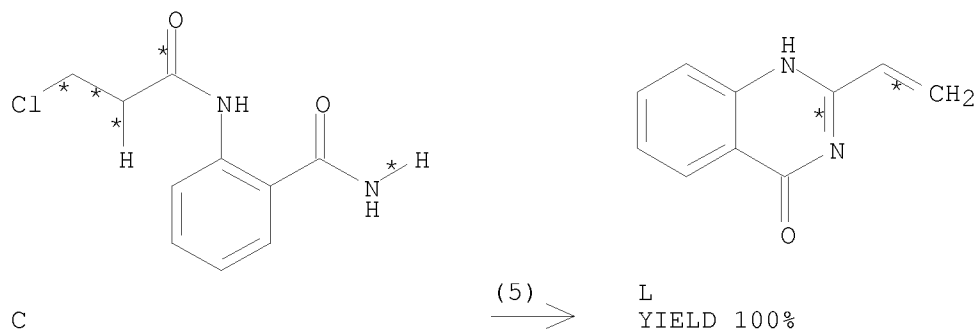
RX(2) RCT B 307001-07-6  
RGT E 75-12-7 Formamide  
PRO D 307001-08-7

RX(3) RCT F 544-92-3, D 307001-08-7  
PRO G 307001-09-8  
SOL 127-19-5 AcNMe2

L3 ANSWER 115 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 133:362747 CASREACT  
TITLE: Synthesis and Reactions of some  
2-Vinyl-3H-quinazolin-4-ones  
AUTHOR(S): Witt, A.; Bergman, J.  
CORPORATE SOURCE: Department of Biosciences, Unit for Organic Chemistry,  
Novum Research Park, Karolinska Institute and  
Sodertorn University College, Huddinge, SE-141 57,  
Swed.  
SOURCE: Tetrahedron (2000), 56(37), 7245-7253  
CODEN: TETRAB; ISSN: 0040-4020  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB A simple, high-yielding synthesis of 2-vinyl-3H-quinazolin-4-one,  
2-(1-chlorovinyl)-3H-quinazolin-4-one, and  
2-(1-bromovinyl)-3H-quinazolin-4-one is reported. The  
2-vinylquinazolinones participate readily in nucleophilic addition reactions.  
Treatment with both carbon and nitrogen nucleophiles results in a clean  
conversion into a variety of 2-substituted 3H-quinazolin-4-one derivs.  
2-(1-Halovinyl)-3H-quinazolin-4-ones reacted with carbon nucleophiles to  
give several derivs. of 2-substituted 3H-quinazolin-4-one.

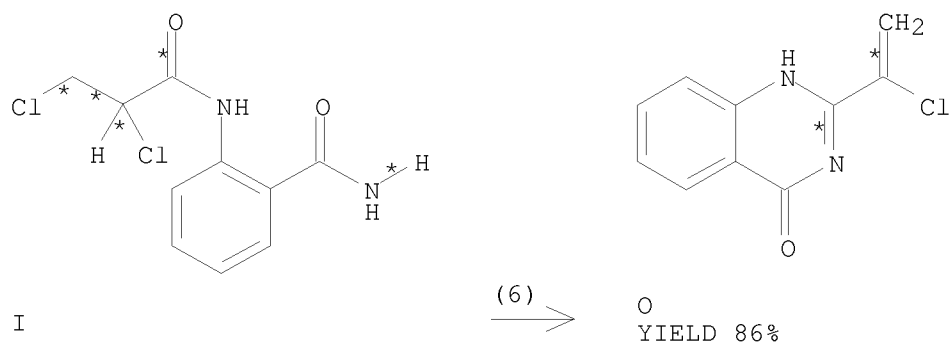
RX(5) OF 72 ...C ==> L...

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RX(5) RCT C 306996-53-2  
RGT M 1310-73-2 NaOH  
PRO L 91634-12-7  
SOL 64-17-5 EtOH

RX(6) OF 72 ...I ==> O...

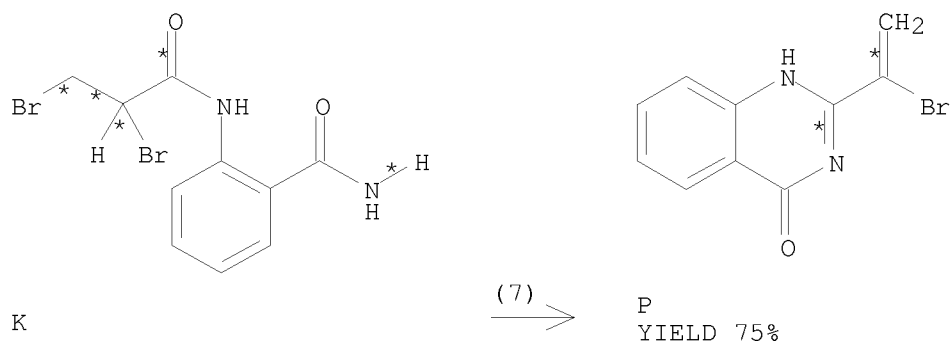


RX(6) RCT I 306996-54-3  
RGT M 1310-73-2 NaOH  
PRO O 306996-56-5  
SOL 64-17-5 EtOH

RX(7) OF 72 ...K ==> P

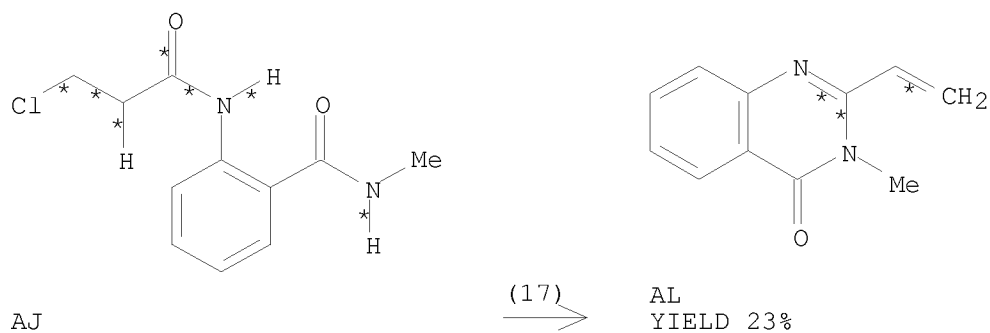


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RX (7) RCT K 306996-55-4  
RGT M 1310-73-2 NaOH  
PRO P 306996-57-6  
SOL 64-17-5 EtOH

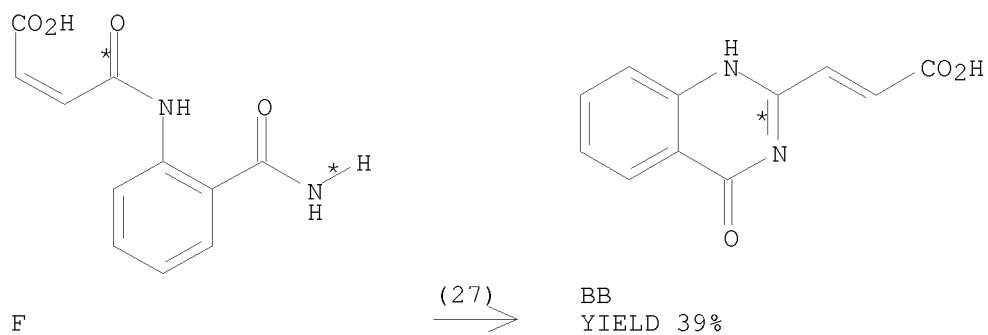
RX (17) OF 72 ...AJ ==> AL...



RX (17) RCT AJ 306996-58-7  
RGT AM 497-19-8 Na<sub>2</sub>CO<sub>3</sub>  
PRO AL 306996-59-8  
SOL 67-56-1 MeOH

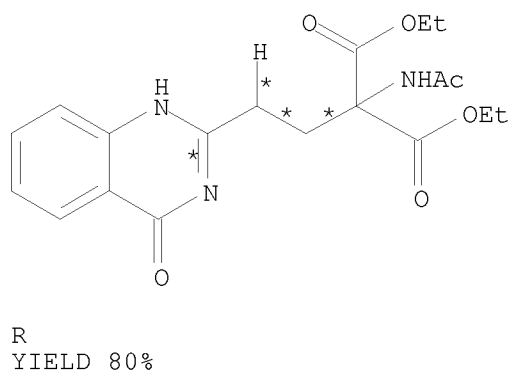
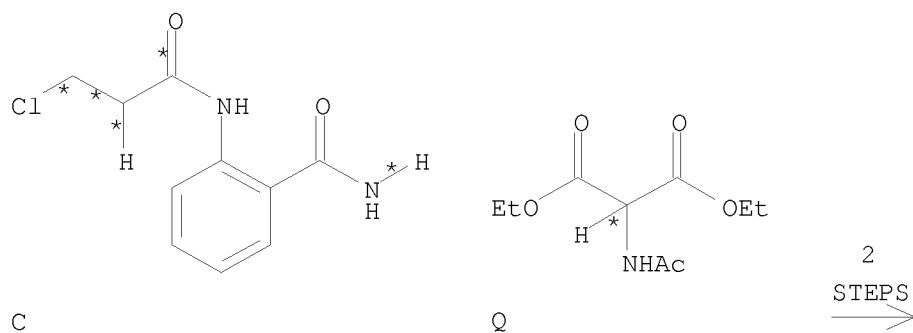
RX (27) OF 72 ...F ==> BB

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RX(27) RCT F 306996-83-8  
RGT BC 127-09-3 AcONa  
PRO BB 306996-85-0  
SOL 108-24-7 Ac2O

RX(32) OF 72 COMPOSED OF RX(5), RX(8)  
RX(32) C + Q  $\implies$  R



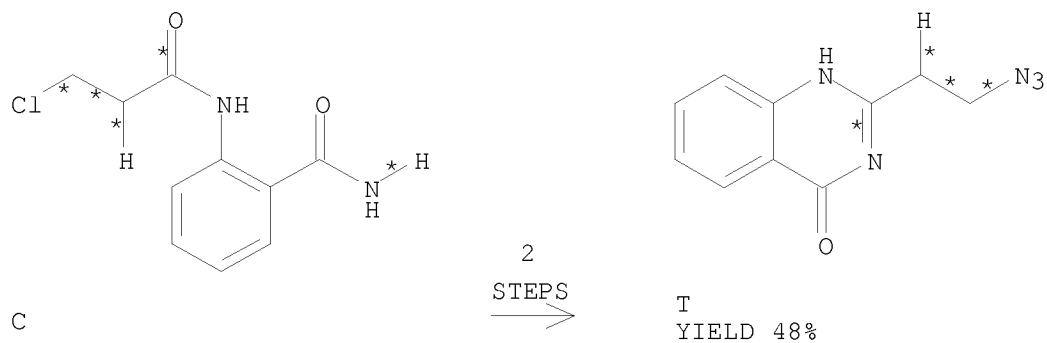
RX(5) RCT C 306996-53-2  
RGT M 1310-73-2 NaOH  
PRO L 91634-12-7

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SOL 64-17-5 EtOH

RX(8) RCT L 91634-12-7, Q 1068-90-2  
RGT S 7440-23-5 Na  
PRO R 306996-62-3  
SOL 64-17-5 EtOH

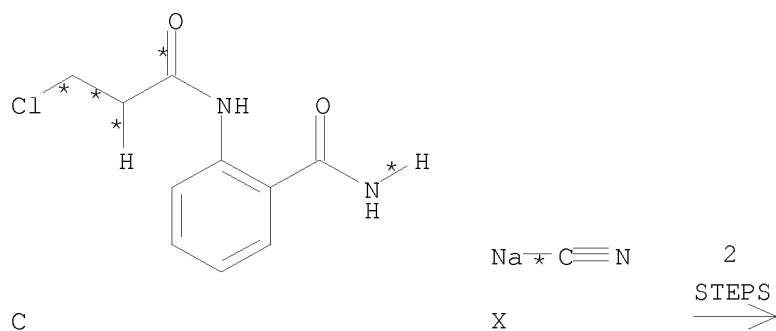
RX(33) OF 72 COMPOSED OF RX(5), RX(9)  
RX(33) C ==> T



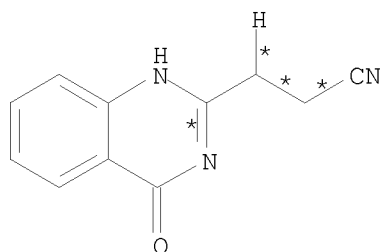
RX(5) RCT C 306996-53-2  
RGT M 1310-73-2 NaOH  
PRO L 91634-12-7  
SOL 64-17-5 EtOH

RX(9) RCT L 91634-12-7  
RGT U 26628-22-8 NaN<sub>3</sub>  
PRO T 306996-66-7  
SOL 109-99-9 THF, 7732-18-5 Water

RX(34) OF 72 COMPOSED OF RX(5), RX(10)  
RX(34) C + X ==> Y



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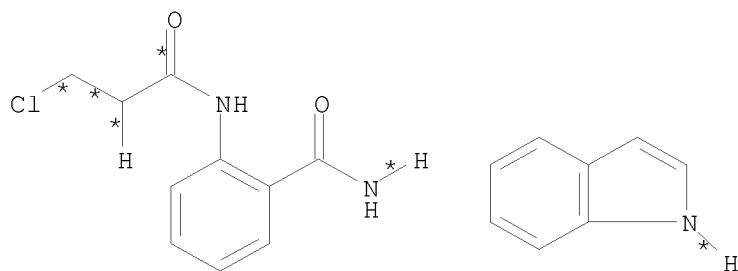


Y  
YIELD 76%

RX(5)        RCT    C 306996-53-2  
              RGT    M 1310-73-2 NaOH  
              PRO    L 91634-12-7  
              SOL    64-17-5 EtOH

RX(10)       RCT    L 91634-12-7, X 143-33-9  
              PRO    Y 1703-02-2  
              SOL    64-17-5 EtOH, 7732-18-5 Water

RX(35) OF 72 COMPOSED OF RX(5), RX(21)  
RX(35)       C    +    AR    ==>    AS

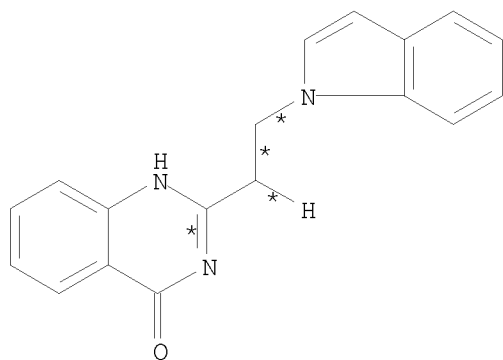


C

AR

2  
STEPS  
→

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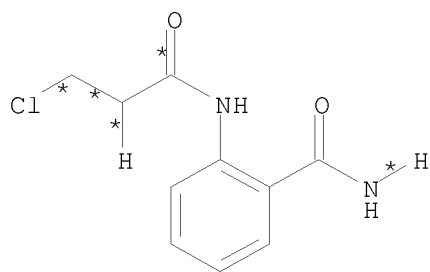


AS  
YIELD 95%

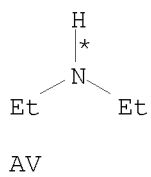
RX(5)      RCT    C   306996-53-2  
              RGT    M   1310-73-2 NaOH  
              PRO    L   91634-12-7  
              SOL    64-17-5 EtOH

RX(21)      RCT    L   91634-12-7, AR 120-72-9  
              PRO    AS   306996-63-4  
              SOL    64-19-7 AcOH

RX(36) OF 72 COMPOSED OF RX(5), RX(23)  
RX(36)      C   +   AV   ==>   AW

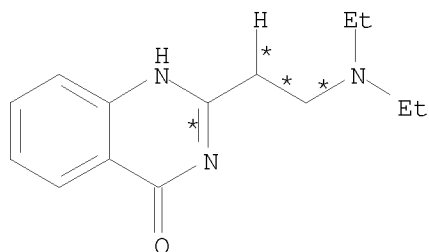


C



2  
STEPS  
→

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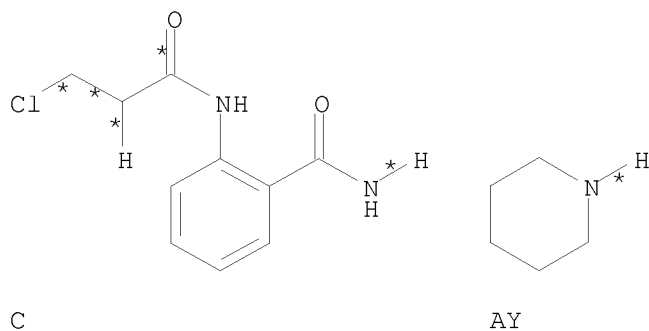


AW  
YIELD 49%

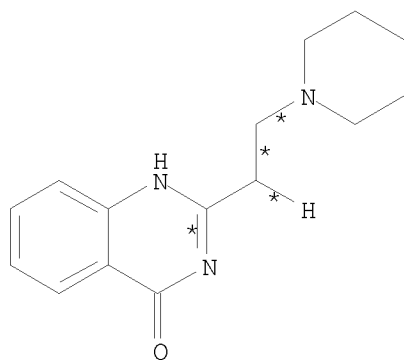
RX(5)        RCT    C 306996-53-2  
              RGT    M 1310-73-2 NaOH  
              PRO    L 91634-12-7  
              SOL    64-17-5 EtOH

RX(23)       RCT    L 91634-12-7, AV 109-89-7  
              RGT    AT 64-19-7 AcOH  
              PRO    AW 95556-34-6  
              SOL    67-56-1 MeOH

RX(37) OF 72 COMPOSED OF RX(5), RX(25)  
RX(37)       C    +    AY    ==>    AZ



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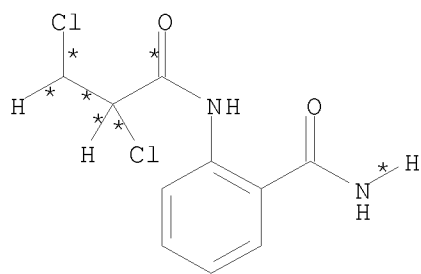


AZ  
YIELD 84%

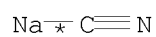
RX(5)      RCT    C 306996-53-2  
             RGT    M 1310-73-2 NaOH  
             PRO    L 91634-12-7  
             SOL    64-17-5 EtOH

RX(25)      RCT    L 91634-12-7, AY 110-89-4  
             RGT    AT 64-19-7 AcOH  
             PRO    AZ 95698-00-3  
             SOL    67-56-1 MeOH

RX(38) OF 72 COMPOSED OF RX(6), RX(11)  
RX(38)      I    +    X    ==>    Z



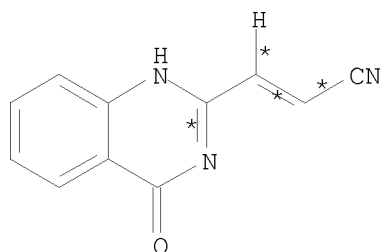
I



X

2  
STEPS  
→

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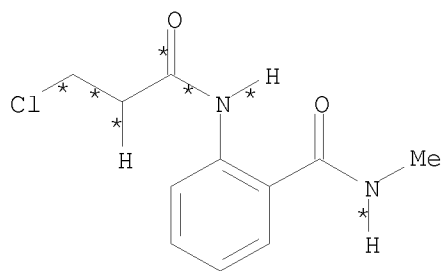


Z  
YIELD 66%

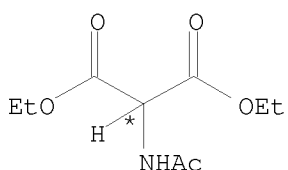
RX(6)      RCT    I 306996-54-3  
              RGT    M 1310-73-2 NaOH  
              PRO    O 306996-56-5  
              SOL    64-17-5 EtOH

RX(11)      RCT    O 306996-56-5, X 143-33-9  
              PRO    Z 306996-81-6  
              SOL    7732-18-5 Water, 64-17-5 EtOH

RX(44) OF 72 COMPOSED OF RX(17), RX(18)  
RX(44)      AJ    +    Q    ==>    AO

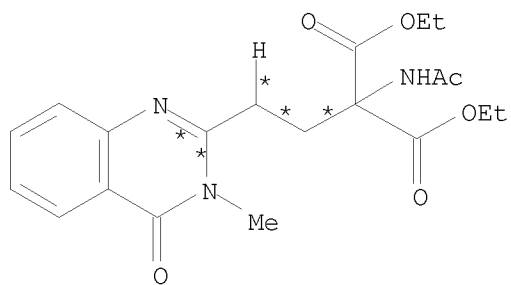


AJ



Q

2  
STEPS  
→



AO  
YIELD 41%

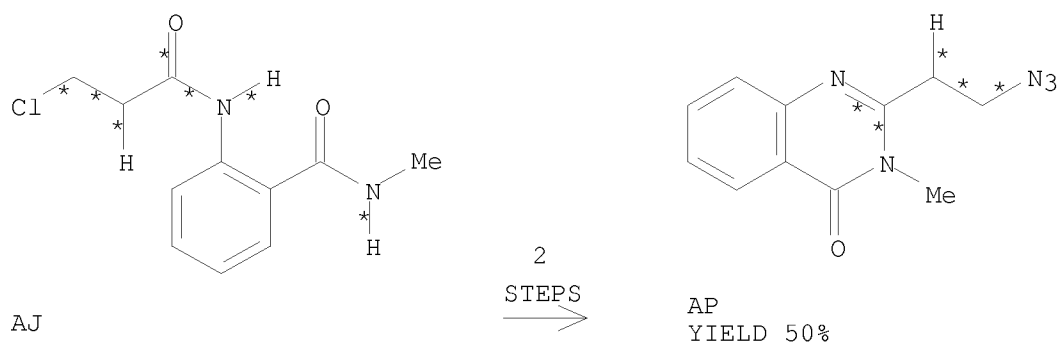


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RX(17)     RCT    AJ 306996-58-7  
             RGT    AM 497-19-8 Na<sub>2</sub>CO<sub>3</sub>  
             PRO    AL 306996-59-8  
             SOL    67-56-1 MeOH

RX(18)     RCT    AL 306996-59-8, Q 1068-90-2  
             RGT    AC 7646-69-7 NaH  
             PRO    AO 306996-69-0  
             SOL    109-99-9 THF

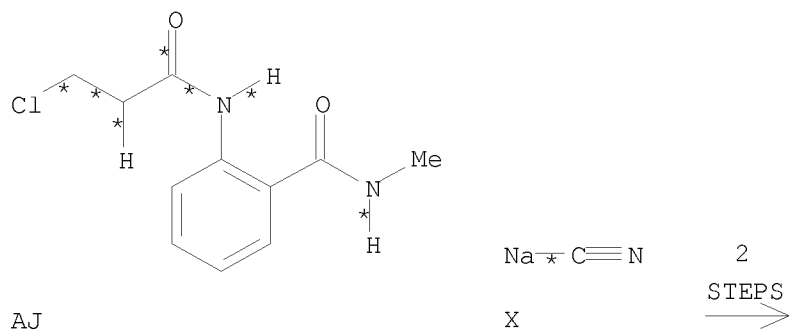
RX(45) OF 72 COMPOSED OF RX(17), RX(19)  
RX(45)     AJ    ==>    AP



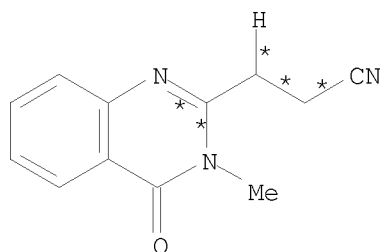
RX(17)     RCT    AJ 306996-58-7  
             RGT    AM 497-19-8 Na<sub>2</sub>CO<sub>3</sub>  
             PRO    AL 306996-59-8  
             SOL    67-56-1 MeOH

RX(19)     RCT    AL 306996-59-8  
             RGT    U 26628-22-8 NaN<sub>3</sub>  
             PRO    AP 306996-77-0  
             SOL    109-99-9 THF, 7732-18-5 Water

RX(46) OF 72 COMPOSED OF RX(17), RX(20)  
RX(46)     AJ    +    X    ==>    AQ



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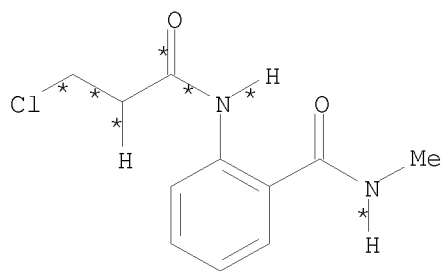


AQ  
YIELD 23%

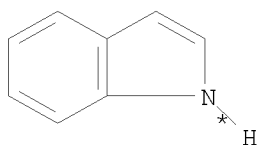
RX(17)      RCT    AJ 306996-58-7  
              RGT    AM 497-19-8 Na<sub>2</sub>CO<sub>3</sub>  
              PRO    AL 306996-59-8  
              SOL    67-56-1 MeOH

RX(20)      RCT    AL 306996-59-8, X 143-33-9  
              PRO    AQ 306996-79-2  
              SOL    64-17-5 EtOH, 7732-18-5 Water

RX(47) OF 72 COMPOSED OF RX(17), RX(22)  
RX(47)      AJ    +    AR    ==>    AU



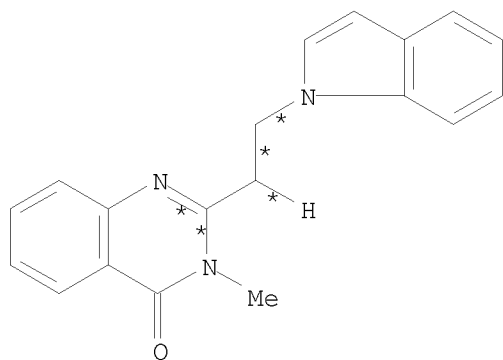
AJ



AR

2  
STEPS  
→

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AU

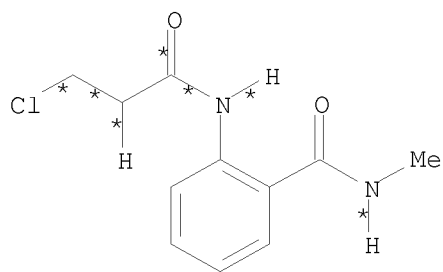
YIELD 75%

RX(17)      RCT    AJ 306996-58-7  
              RGT    AM 497-19-8 Na<sub>2</sub>CO<sub>3</sub>  
              PRO    AL 306996-59-8  
              SOL    67-56-1 MeOH

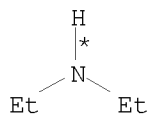
RX(22)      RCT    AL 306996-59-8, AR 120-72-9  
              PRO    AU 306996-71-4  
              SOL    64-19-7 AcOH

RX(48) OF 72 COMPOSED OF RX(17), RX(24)

RX(48)      AJ + AV ==> AX



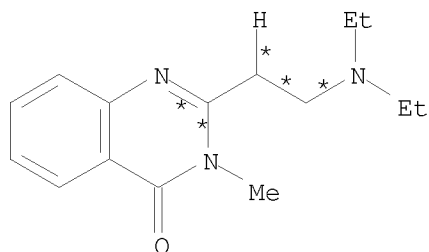
AJ



AV

2  
STEPS  
→

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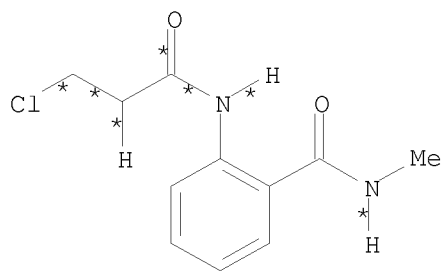


AX  
YIELD 85%

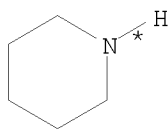
RX(17)      RCT    AJ 306996-58-7  
              RGT    AM 497-19-8 Na<sub>2</sub>CO<sub>3</sub>  
              PRO    AL 306996-59-8  
              SOL    67-56-1 MeOH

RX(24)      RCT    AL 306996-59-8, AV 109-89-7  
              RGT    AT 64-19-7 AcOH  
              PRO    AX 306996-73-6  
              SOL    67-56-1 MeOH

RX(49) OF 72 COMPOSED OF RX(17), RX(26)  
RX(49)      AJ    +    AY    ==>    BA

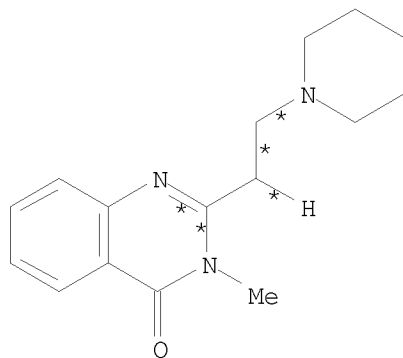


AJ



AY

2  
STEPS  
→



BA  
YIELD 99%

RX(17) RCT AJ 306996-58-7  
RGT AM 497-19-8 Na<sub>2</sub>CO<sub>3</sub>  
PRO AL 306996-59-8  
SOL 67-56-1 MeOH

RX(26) RCT AL 306996-59-8, AY 110-89-4  
RGT AT 64-19-7 AcOH  
PRO BA 306996-75-8  
SOL 67-56-1 MeOH

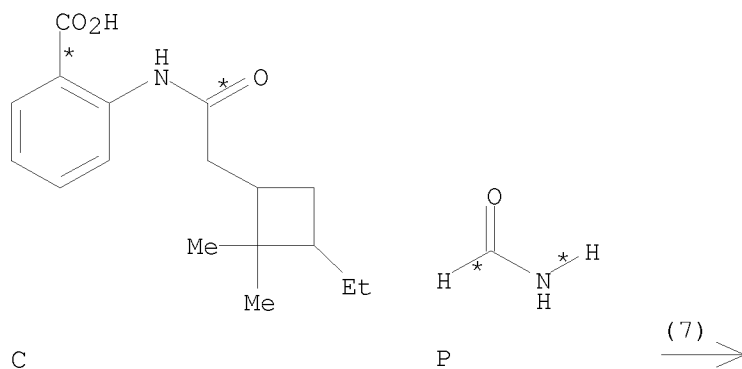
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 116 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 132:180542 CASREACT  
TITLE: 2-[(3-Ethyl-2,2-dimethylcyclobutyl)methyl]-4(3H)-quinazolinones  
AUTHOR(S): Avotin'sh, F. M.; Petrova, M. V.; Pastors, P. V.; Strakov, A. Ya.  
CORPORATE SOURCE: Riga Technical University, Riga, LV-1658, Latvia  
SOURCE: Chemistry of Heterocyclic Compounds (New York) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (1999), 35(6), 722-728  
CODEN: CHCCAL; ISSN: 0009-3122  
PUBLISHER: Consultants Bureau  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Anthranilic acid and its 5-bromo and 4-chloro derivs. react with pinanoic and pinonoic acid chlorides to give the corresponding N-acyl derivs. The pinanoyl derivs. give the title compds. when refluxed in formamide. Pinanoylanthranilic acid reacts with dicyclohexylcarbodiimide to give 2-[(3-ethyl-2,2-dimethylcyclobutyl)methyl]benz-3,1-oxazin-4(H)-one and subsequently with hydrazine hydrate to give 3-amino-2-[(3-ethyl-2,2-dimethylcyclobutyl)methyl]-4(3H)-quinazolinone. Refluxing the pinanoyl- and pinonoylanthranilic acids with acetic anhydride gives acetylanthranilic acid, and pinonoylanthranilic acid gives 4(3H)-quinazolinone with formamide.

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RX(7) OF 22      ...C + P ==> Q



Q  
YIELD 70%

RX(7)      RCT   C 259262-82-3, P 75-12-7

STAGE(1)

STAGE(2)

RGT   R 144-55-8 NaHCO<sub>3</sub>

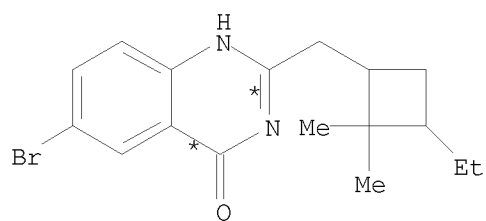
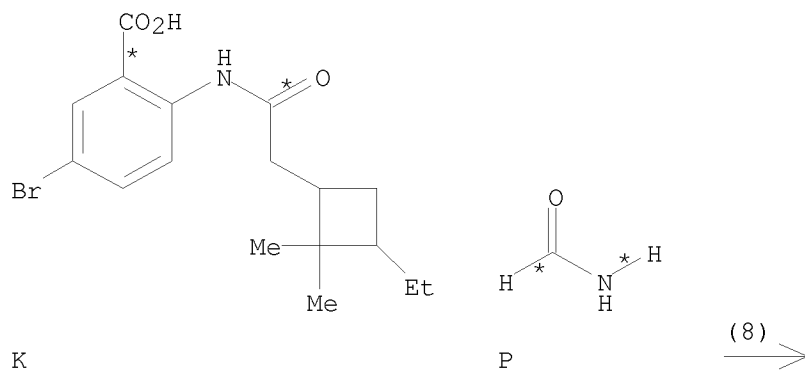
SOL   7732-18-5 Water

PRO   Q 259262-90-3

NTE   first stage thermal without solvent

RX(8) OF 22      ...K + P ==> S

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S  
YIELD 93%

RX(8) RCT K 259262-83-4, P 75-12-7

STAGE(1)

STAGE(2)

RGT R 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water

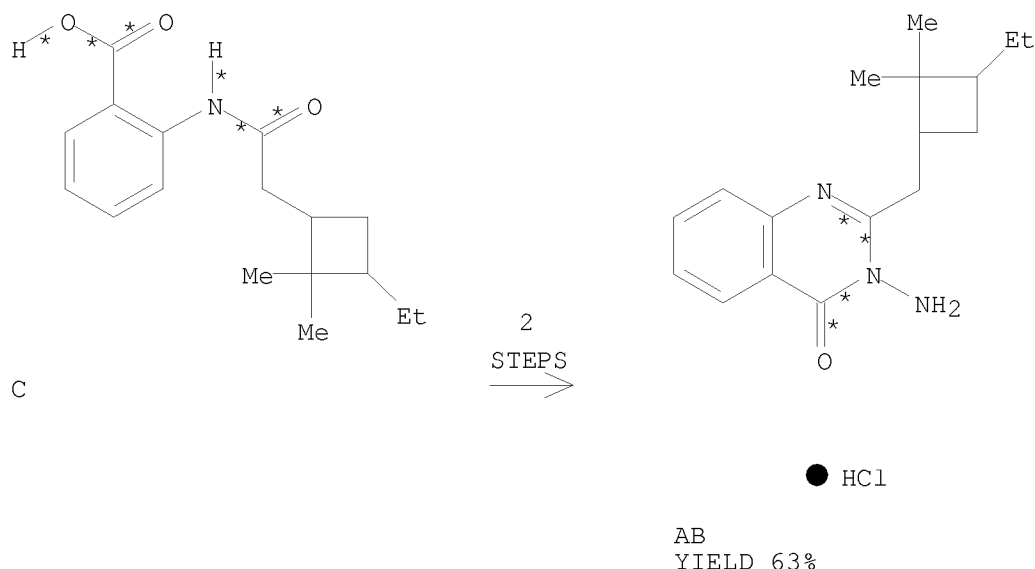
PRO S 259262-91-4

NTE first stage thermal without solvent

RX(20) OF 22 COMPOSED OF RX(12), RX(13)

RX(20) C ==> AB

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RX(12) RCT C 259262-82-3  
RGT AA 538-75-0 DCC  
PRO Z 259262-93-6  
SOL 71-43-2 Benzene

RX(13) RCT Z 259262-93-6

STAGE(1)

RGT AC 302-01-2 N2H4  
SOL 110-86-1 Pyridine

STAGE(2)

RGT E 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO AB 259262-94-7

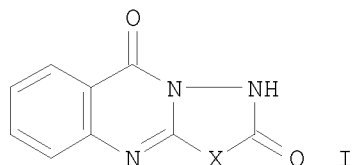
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 117 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 131:286478 CASREACT  
TITLE: Transformations of diacyl derivatives of anthranilic hydrazide under cyclodehydration conditions  
AUTHOR(S): Shemchuk, L. A.; Chernykh, V. P.; Ivanova, I. L.; Snitkovskii, E. L.; Zhirov, M. V.; Turov, A. V.  
CORPORATE SOURCE: Ukrainian Pharmaceutical Academy, Kharkov, 10002, Ukraine  
SOURCE: Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (1999), 35(2), 286-289  
CODEN: RJOCEQ; ISSN: 1070-4280  
PUBLISHER: MAIK Nauka/Interperiodica Publishing  
DOCUMENT TYPE: Journal



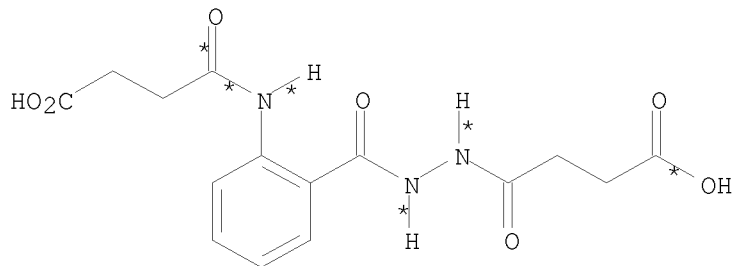
10/ 562,112

LANGUAGE: English  
GI



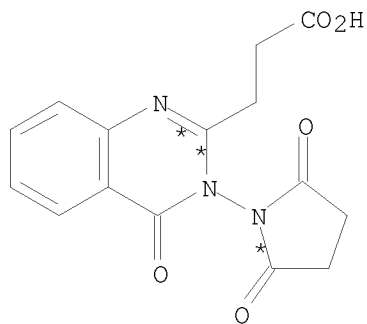
AB Acylation of anthranilic hydrazide with anhydrides of dicarboxylic acids afforded succinic N'-[2-(3-carboxypropionylamino)benzoyl]hydrazide, glutaric N'-[2-(4-carboxybutyrylamino)benzoyl]hydrazide, and phthalic N'-[2-(2-carboxybenzoylamino)benzoyl]hydrazide. Heating these compds. in acetic anhydride with sodium acetate yielded the corresponding diimides. Thermolysis of the diacyl derivs. of the anthranilic hydrazides containing succinic and phthalic moieties furnished, resp., 3,4-dihydropyridazino[2,3-b]quinazoline-2,10-dione (I, X = CH<sub>2</sub>CH<sub>2</sub>) and phthalazino[1,2-b]quinazoline-2,12-dione (I, X = o-C<sub>6</sub>H<sub>4</sub>). In acetic acid diimides or derivs. of 4-quinazolinone were formed, depending on the nature of the dicarboxylic acid.

RX(11) OF 18 ...C ==> T



C

(11)  $\longrightarrow$



T  
YIELD 51%

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RX(11) RCT C 245724-38-3

STAGE(1)

RGT O 64-19-7 AcOH

STAGE(2)

RGT L 7732-18-5 Water

PRO T 245724-45-2

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 118 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 131:129961 CASREACT

TITLE: Synthesis and reactions of  
2-[2-(2,4,6-trimethylbenzoyl)vinyl]-4H-3,1-benzoxazin-  
4-one and antimicrobial activity

AUTHOR(S): Abdel-Fattah, M. E.; Soliman, E. A.; Soliman, S. M. A.

CORPORATE SOURCE: Chemistry Department, Faculty of Science, Suez Canal

University Ismailia, Cairo, Egypt

SOURCE: Indian Journal of Heterocyclic Chemistry (1999), 8(3),  
177-182

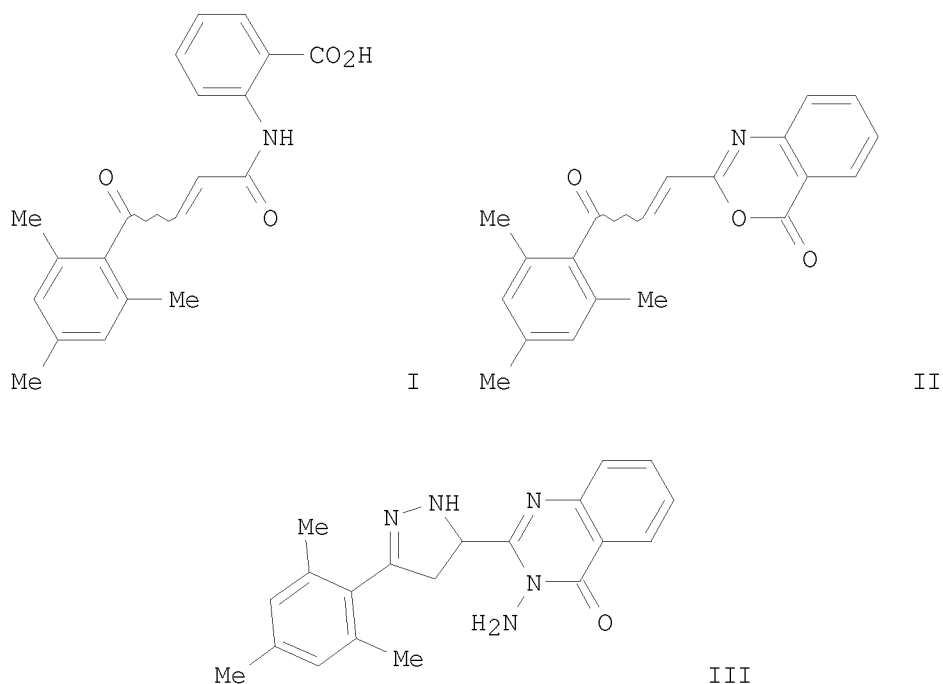
CODEN: IJCHEI; ISSN: 0971-1627

PUBLISHER: Prof. R. S. Varma

DOCUMENT TYPE: Journal

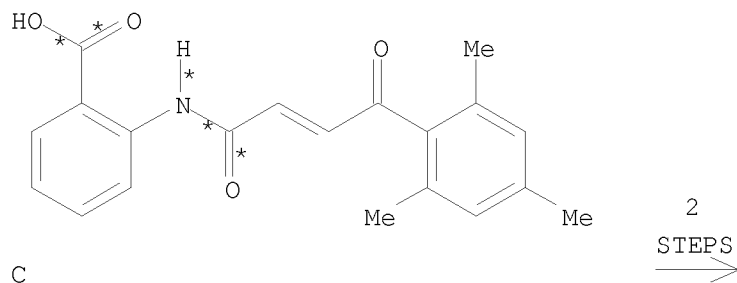
LANGUAGE: English

GI

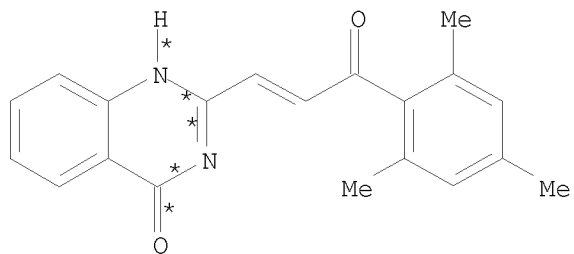


AB  $\beta$ -(2,4,6-Trimethylbenzoyl)-acryloyl chloride reacts with anthranilic acid to give adduct I which is cyclized by the action of acetic anhydride to give the benzoxazinone II. Condensation of II with hydrazine hydrate gave pyrazole III. The behavior of III towards aromatic aldehydes, ketones, phthalic Anhydride, and amino acid chlorides has been investigated. Reaction of II with o-phenylenediamine, ammonia, Grignard reagents, Friedel-Crafts reaction and bromine has been described. Some of the compds. were tested for antibacterial activity; some were active against gram-neg. and gram-pos. bacterial.

RX(31) OF 87 COMPOSED OF RX(2), RX(6)  
 RX(31) C ==> O



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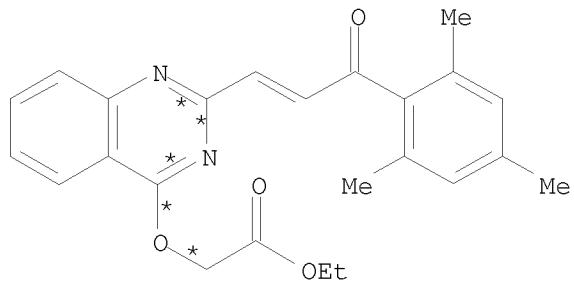
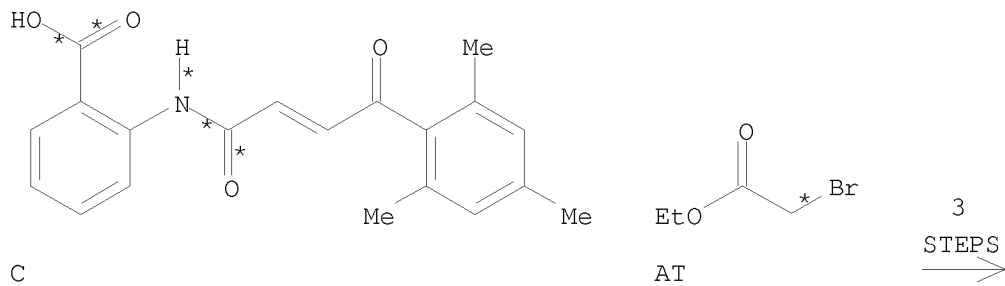


O

RX (2)	RCT	C	234103-28-7
	PRO	E	234103-30-1
	SOL		108-24-7 Ac2O

RX (6)	RCT	E	234103-30-1
	RGT	P	7664-41-7 NH3
	PRO	O	234103-64-1
	SOL		64-17-5 EtOH

RX(72) OF 87 COMPOSED OF RX(2), RX(6), RX(21)

$$\text{RX(72)} \quad \text{C} + \text{AT} \implies \text{AU}$$


AU

RX (2)	RCT	C	234103-28-7
	PRO	E	234103-30-1
	SOL		108-24-7 Ac2O

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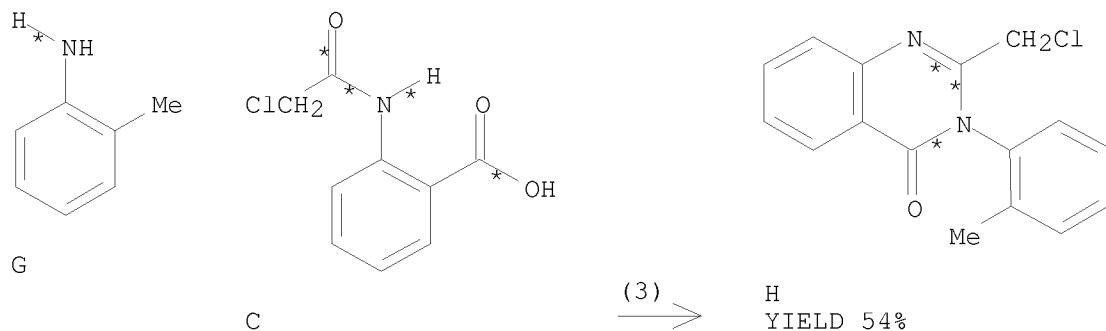
RX(6) RCT E 234103-30-1  
RGT P 7664-41-7 NH3  
PRO O 234103-64-1  
SOL 64-17-5 EtOH

RX(21) RCT O 234103-64-1, AT 105-36-2  
RGT AV 584-08-7 K2CO3  
PRO AU 234103-66-3  
SOL 67-64-1 Me2CO

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 119 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 130:311760 CASREACT  
TITLE: Synthesis and fungicidal activity of 3-aryl-2-(4'-arylthiazol-2'-ylaminomethyl) quinazol-4 (3H)-ones  
AUTHOR(S): Pattanaik, J. M.; Pattanaik, M.; Bhatta, D.  
CORPORATE SOURCE: Department of Chemistry, Utkal University, Bhubaneswar, 751 004, India  
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1998), 37B(12), 1304-1306  
CODEN: IJSBDB; ISSN: 0376-4699  
PUBLISHER: National Institute of Science Communication, CSIR  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB A series of 3-aryl-2-(4-aryl-2-thiazolylaminomethyl) quinazol-4(3H)-ones was prepared by condensing 3-aryl-2-chloromethylquinazol-4(3H)-ones with 2-amino-4-substituted phenylthiazoles. Another group of 3-aryl-6,8-dibromo-2-(4-aryl-2-thiazolylaminomethyl)quinazol-4(3H)-ones was also synthesized from 3-aryl-6,8-dibromo-2-chloromethylquinazol-4(3H)-ones and 2-amino-4-substituted phenylthiazoles in the same manner. Their antifungal activity was determined

RX(3) OF 106 ...G + C ==> H...

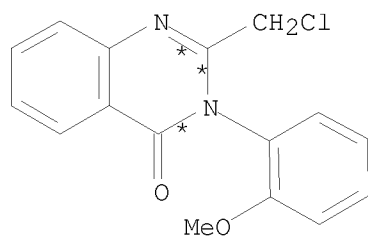
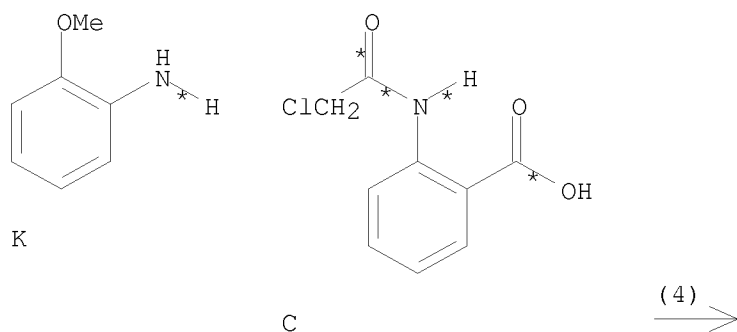


RX(3) RCT G 95-53-4, C 14422-49-2  
RGT I 584-08-7 K2CO3  
PRO H 3166-54-9

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SOL 64-17-5 EtOH  
NTE 6 H

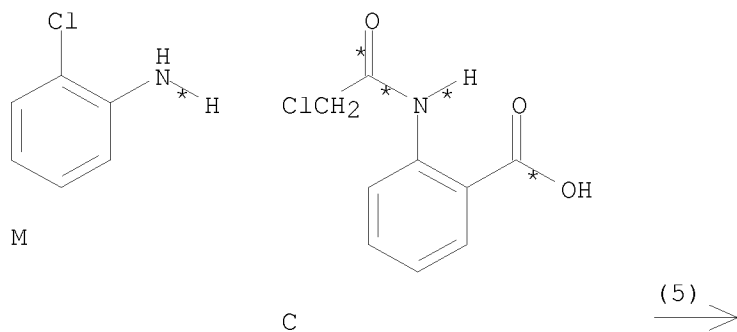
RX(4) OF 106 ...K + C ==> L...



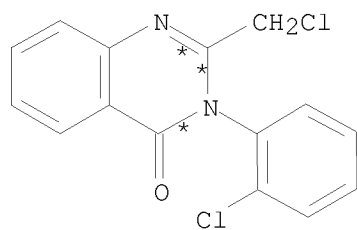
L  
YIELD 54%

RX(4) RCT K 90-04-0, C 14422-49-2  
RGT I 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO L 22312-81-8  
SOL 64-17-5 EtOH  
NTE 6 H

RX(5) OF 106 ...M + C ==> N...



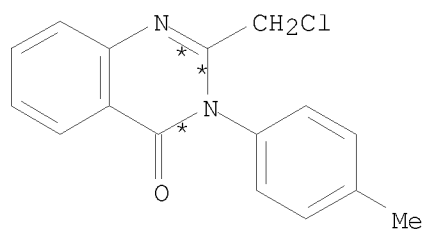
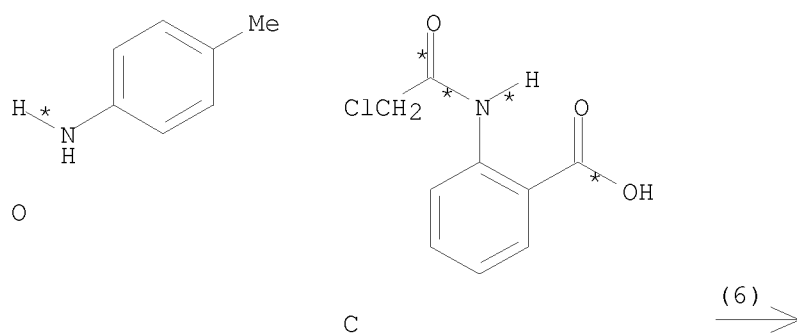
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N  
YIELD 54%

RX(5)        RCT    M 95-51-2, C 14422-49-2  
               RGT    I 584-08-7 K2CO3  
               PRO    N 22312-83-0  
               SOL    64-17-5 EtOH  
               NTE    6 H

RX(6) OF 106        ...O + C ==> P...



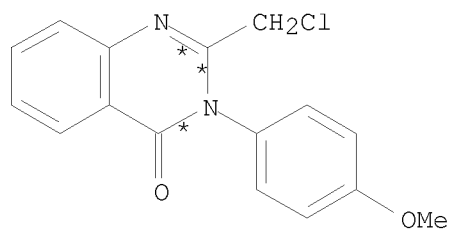
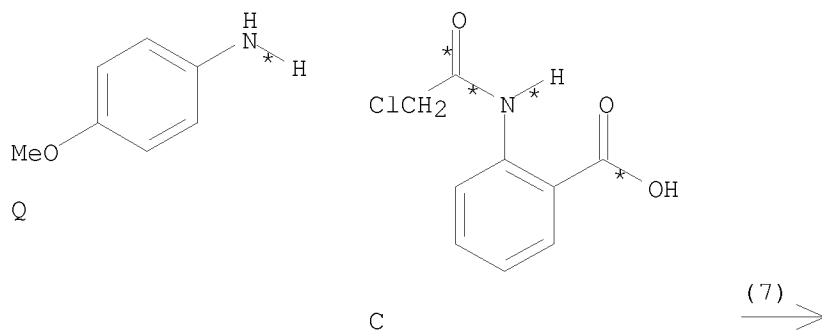
P  
YIELD 54%

RX(6)        RCT    O 106-49-0, C 14422-49-2  
               RGT    I 584-08-7 K2CO3  
               PRO    P 22312-80-7

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SOL 64-17-5 EtOH  
NTE 6 H

RX(7) OF 106 ...Q + C ==> R...



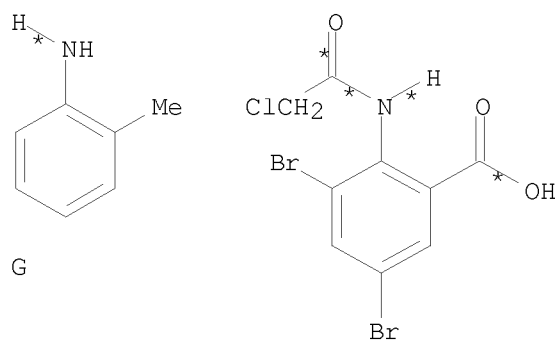
R  
YIELD 54%

RX(7) RCT Q 104-94-9, C 14422-49-2  
RGT I 584-08-7 K2CO3  
PRO R 22312-82-9  
SOL 64-17-5 EtOH  
NTE 6 H

RX(8) OF 106 ...G + F ==> S...



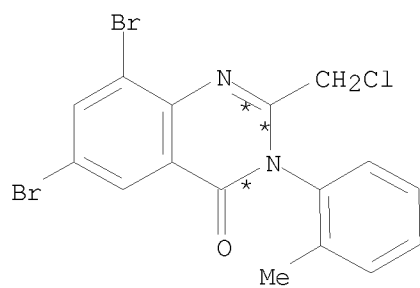
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G

F

(8)  $\longrightarrow$

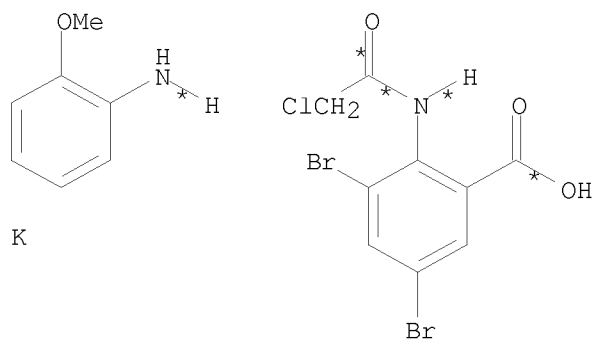


S

YIELD 59%

RX(8)      RCT    G 95-53-4, F 103952-88-1  
              RGT    I 584-08-7 K2CO3  
              PRO    S 177167-07-6  
              SOL    64-17-5 EtOH  
              NTE    6 H

RX(9) OF 106      ...K + F ==> T...

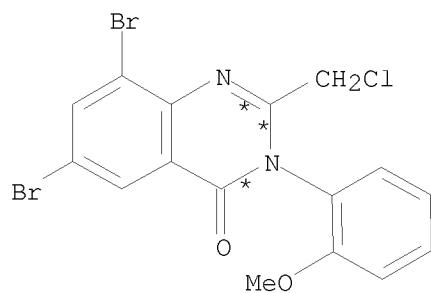


K

F

(9)  $\longrightarrow$

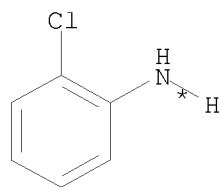
10/ 562,112



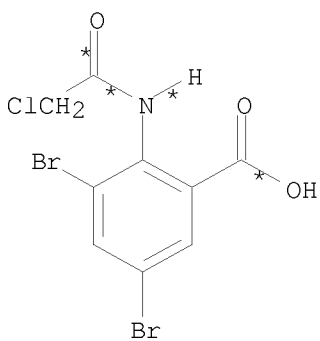
T  
YIELD 54%

RX(9)        RCT   K 90-04-0, F 103952-88-1  
               RGT   I 584-08-7 K2CO3  
               PRO   T 104308-99-8  
               SOL   64-17-5 EtOH  
               NTE   6 H

RX(10) OF 106        ...M + F ==> U...



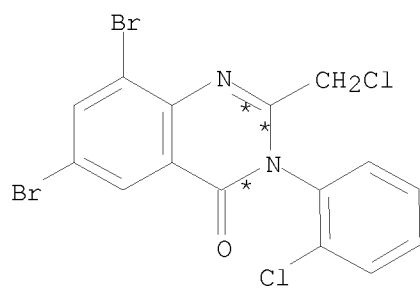
M



F

(10) >

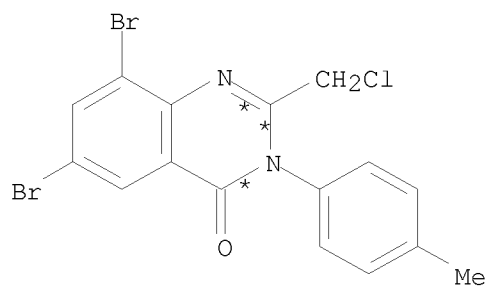
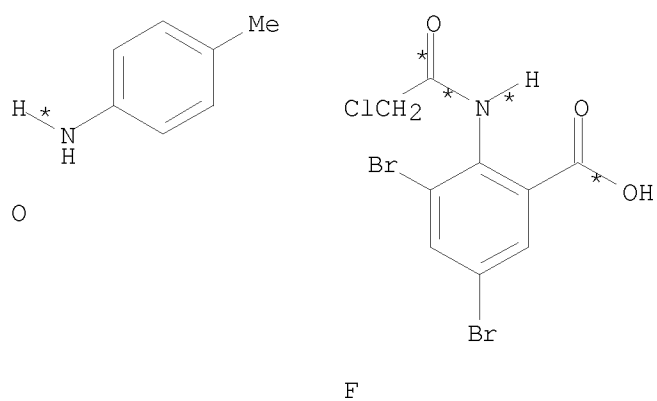
10/ 562,112



U  
YIELD 54%

RX(10)      RCT    M 95-51-2, F 103952-88-1  
               RGT    I 584-08-7 K2CO3  
               PRO    U 104308-98-7  
               SOL    64-17-5 EtOH  
               NTE    6 H

RX(11) OF 106      ...O + F ==> V...

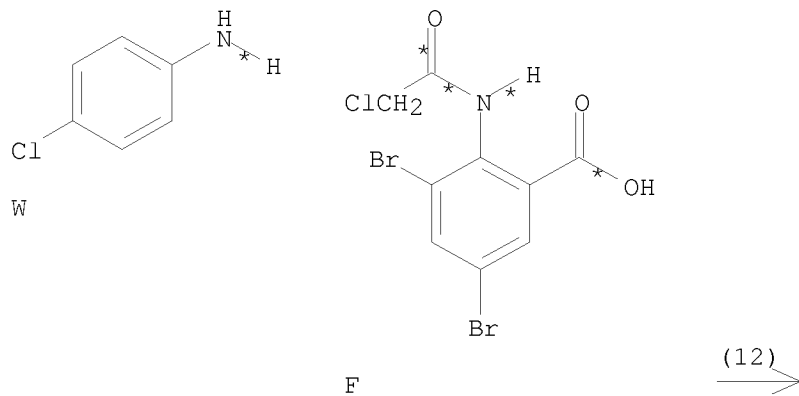


V  
YIELD 54%

10/ 562,112

RX(11)      RCT   O 106-49-0, F 103952-88-1  
             RGT   I 584-08-7 K2CO3  
             PRO   V 103952-89-2  
             SOL   64-17-5 EtOH  
             NTE   6 H

RX(12) OF 106      ...W + F ==> X...

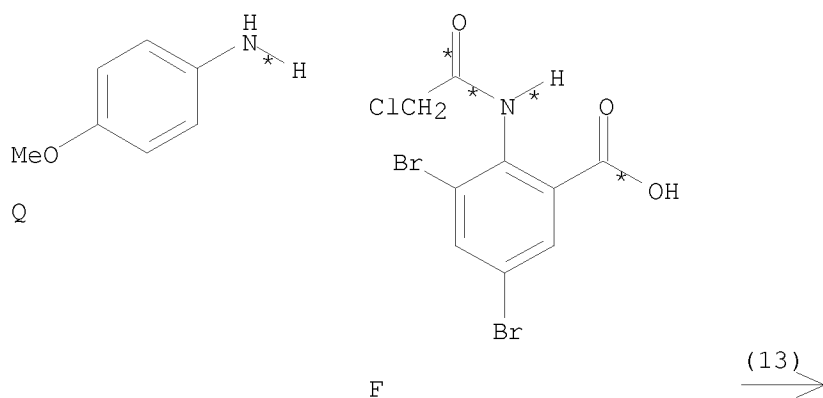


X  
YIELD 54%

RX(12)      RCT   W 106-47-8, F 103952-88-1  
             RGT   I 584-08-7 K2CO3  
             PRO   X 223590-80-5  
             SOL   64-17-5 EtOH  
             NTE   6 H

RX(13) OF 106      ...Q + F ==> Y...

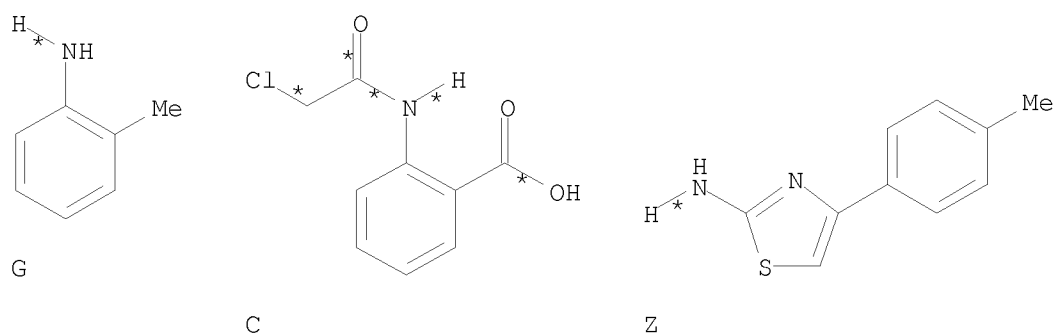
10/ 562,112



Y  
YIELD 54%

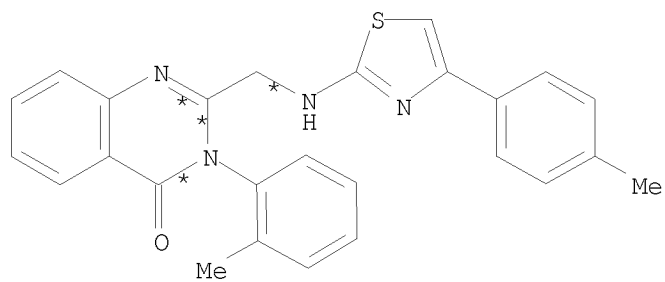
RX(13)     RCT   Q 104-94-9, F 103952-88-1  
              RGT   I 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
              PRO   Y 223590-81-6  
              SOL   64-17-5 EtOH  
              NTE   6 H

RX(57) OF 106 COMPOSED OF RX(3), RX(16)  
 RX(57)     G + C + Z ==> AE



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2  
STEPS  
→

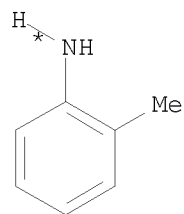


AE  
YIELD 56%

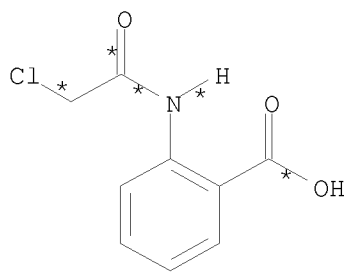
RX(3) RCT G 95-53-4, C 14422-49-2  
RGT I 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO H 3166-54-9  
SOL 64-17-5 EtOH  
NTE 6 H

RX(16) RCT Z 2103-91-5, H 3166-54-9  
RGT B 110-86-1 Pyridine  
PRO AE 223590-50-9  
NTE 4 H

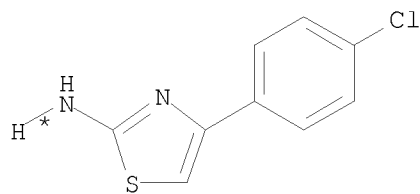
RX(58) OF 106 COMPOSED OF RX(3), RX(17)  
RX(58) G + C + AC ==> AF



G



C

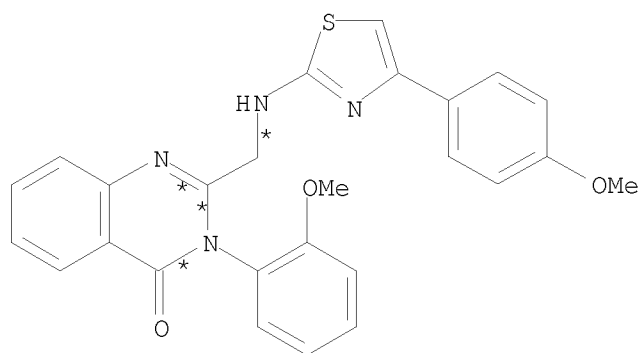


AC

2  
STEPS  
→



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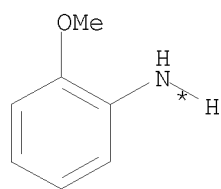


AH  
YIELD 52%

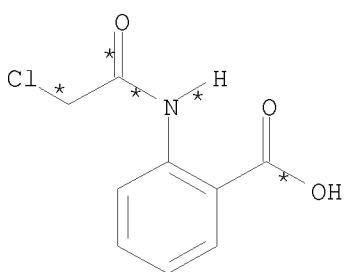
RX(4)      RCT    K 90-04-0, C 14422-49-2  
             RGT    I 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
             PRO    L 22312-81-8  
             SOL    64-17-5 EtOH  
             NTE    6 H

RX(18)     RCT    AG 2104-04-3, L 22312-81-8  
             RGT    B 110-86-1 Pyridine  
             PRO    AH 223590-52-1  
             NTE    4 H

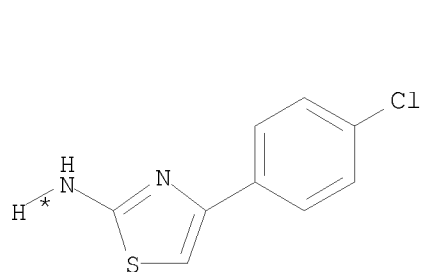
RX(60) OF 106 COMPOSED OF RX(4), RX(19)  
RX(60)      K + C + AC ==> AI



K



C

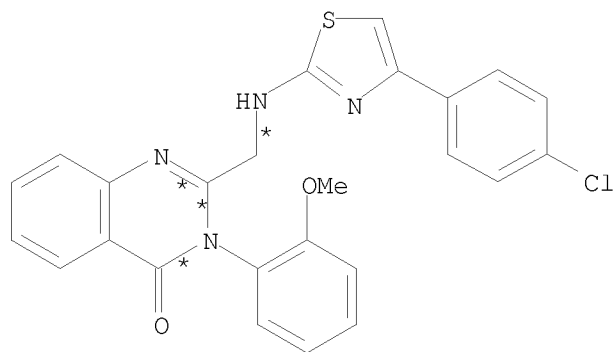


AC

2  
STEPS  
→



10/ 562,112

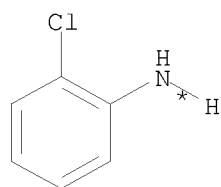


AI  
YIELD 60%

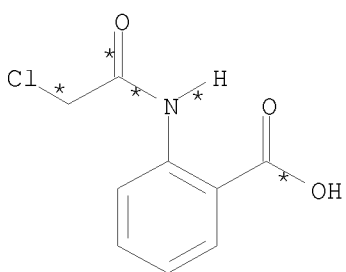
RX(4) RCT K 90-04-0, C 14422-49-2  
RGT I 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO L 22312-81-8  
SOL 64-17-5 EtOH  
NTE 6 H

RX(19) RCT AC 2103-99-3, L 22312-81-8  
RGT B 110-86-1 Pyridine  
PRO AI 223590-53-2  
NTE 4 H

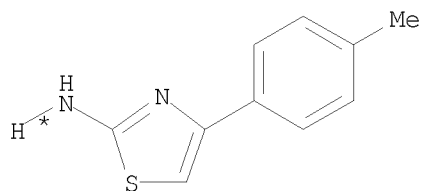
RX(61) OF 106 COMPOSED OF RX(5), RX(20)  
RX(61) M + C + Z ==> AJ



M



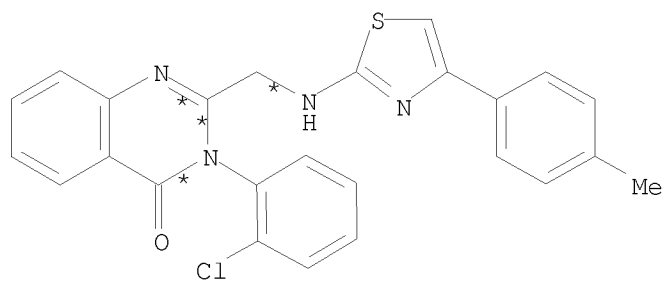
C



Z

2  
STEPS  
→

10/ 562,112

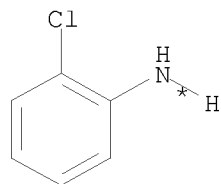


AJ  
YIELD 56%

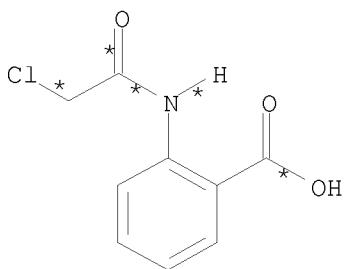
RX(5)        RCT    M 95-51-2, C 14422-49-2  
              RGT    I 584-08-7 K2CO3  
              PRO    N 22312-83-0  
              SOL    64-17-5 EtOH  
              NTE    6 H

RX(20)       RCT    Z 2103-91-5, N 22312-83-0  
              RGT    B 110-86-1 Pyridine  
              PRO    AJ 223590-54-3  
              NTE    4 H

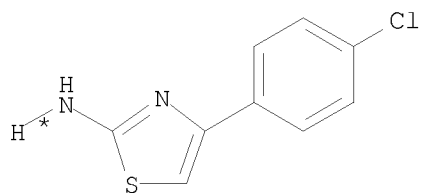
RX(62) OF 106 COMPOSED OF RX(5), RX(21)  
RX(62)       M + C + AC ==> AK



M



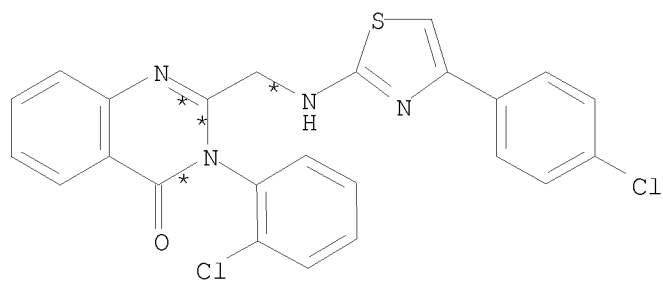
C



AC

2  
STEPS  
→

10/ 562,112

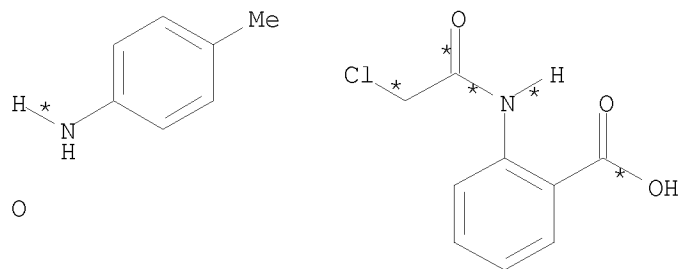


AK  
YIELD 57%

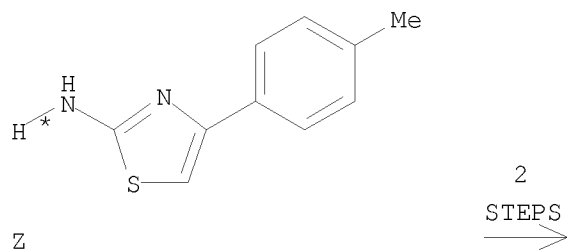
RX(5) RCT M 95-51-2, C 14422-49-2  
RGT I 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO N 22312-83-0  
SOL 64-17-5 EtOH  
NTE 6 H

RX(21) RCT AC 2103-99-3, N 22312-83-0  
RGT B 110-86-1 Pyridine  
PRO AK 223590-55-4  
NTE 4 H

RX(63) OF 106 COMPOSED OF RX(6), RX(22)  
RX(63) O + C + Z ==> AL

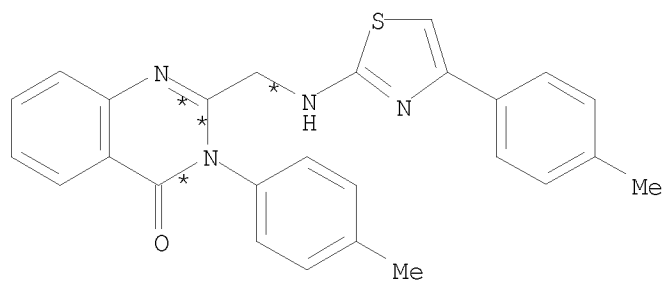


C



2  
STEPS  
→

10/ 562,112

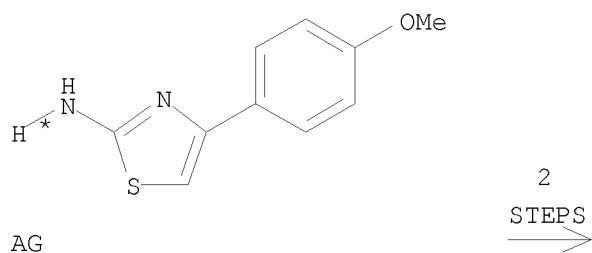
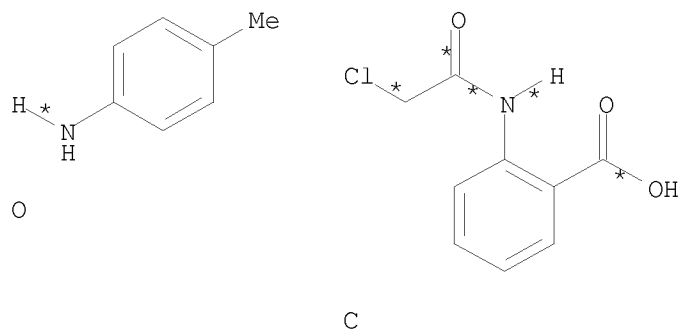


AL  
YIELD 58%

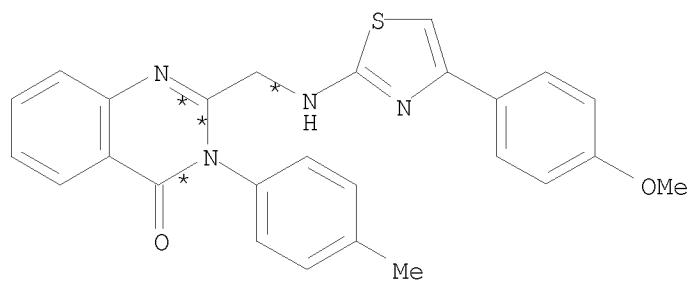
RX(6) RCT O 106-49-0, C 14422-49-2  
RGT I 584-08-7 K2CO3  
PRO P 22312-80-7  
SOL 64-17-5 EtOH  
NTE 6 H

RX(22) RCT Z 2103-91-5, P 22312-80-7  
RGT B 110-86-1 Pyridine  
PRO AL 223590-56-5  
NTE 4 H

RX(64) OF 106 COMPOSED OF RX(6), RX(23)  
RX(64) O + C + AG ==> AM



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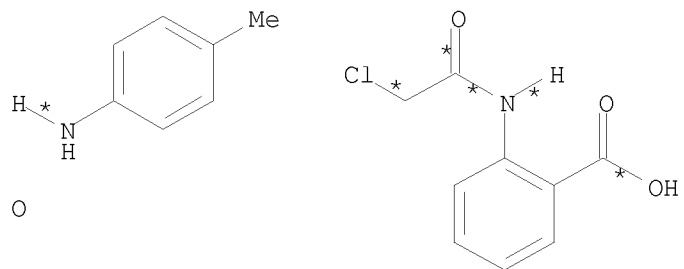


AM  
YIELD 52%

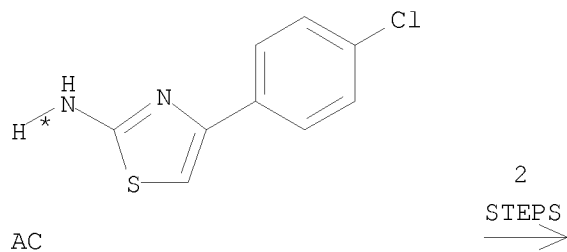
RX(6)      RCT    O 106-49-0, C 14422-49-2  
              RGT    I 584-08-7 K2CO3  
              PRO    P 22312-80-7  
              SOL    64-17-5 EtOH  
              NTE    6 H

RX(23)      RCT    AG 2104-04-3, P 22312-80-7  
              RGT    B 110-86-1 Pyridine  
              PRO    AM 223590-57-6  
              NTE    4 H

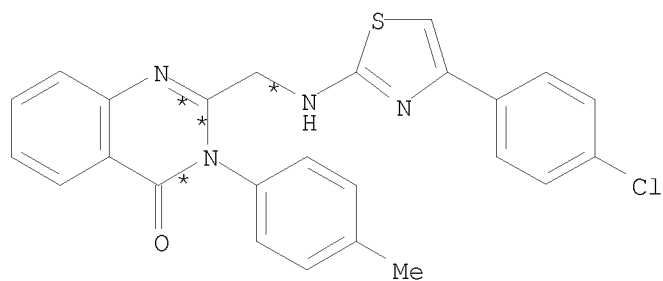
RX(65) OF 106 COMPOSED OF RX(6), RX(24)  
RX(65)      O + C + AC ==> AN



C



10/ 562,112

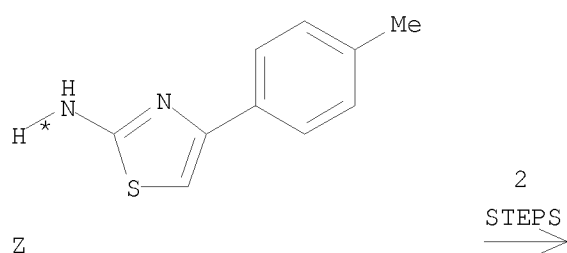
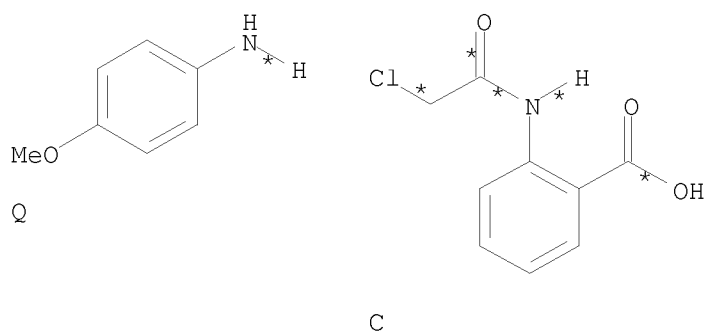


AN  
YIELD 48%

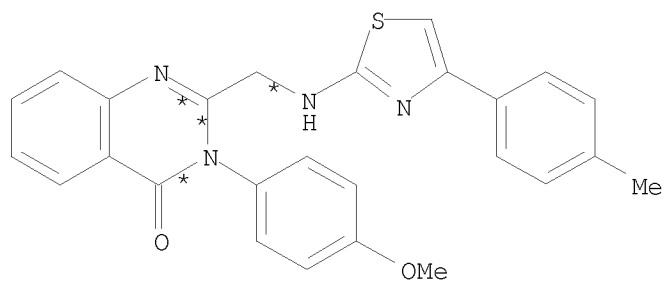
RX(6)      RCT    O 106-49-0, C 14422-49-2  
              RGT    I 584-08-7 K2CO3  
              PRO    P 22312-80-7  
              SOL    64-17-5 EtOH  
              NTE    6 H

RX(24)     RCT    AC 2103-99-3, P 22312-80-7  
              RGT    B 110-86-1 Pyridine  
              PRO    AN 223590-58-7  
              NTE    4 H

RX(66) OF 106 COMPOSED OF RX(7), RX(28)  
 RX(66)      Q + C + Z ==> AS



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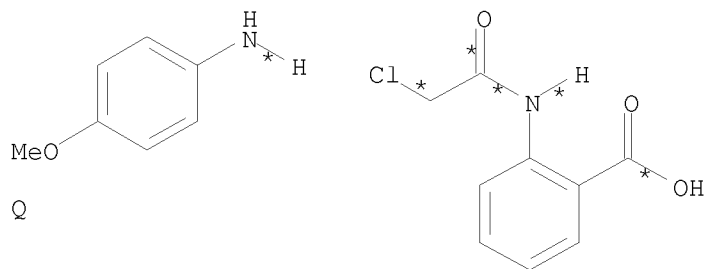


AS  
YIELD 51%

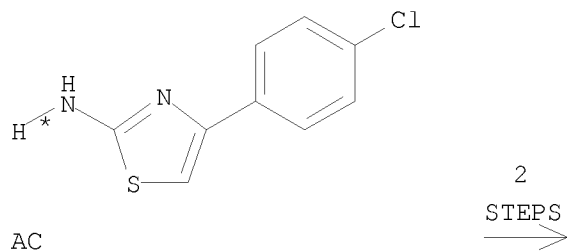
RX(7)      RCT    Q 104-94-9, C 14422-49-2  
              RGT    I 584-08-7 K2CO3  
              PRO    R 22312-82-9  
              SOL    64-17-5 EtOH  
              NTE    6 H

RX(28)     RCT    Z 2103-91-5, R 22312-82-9  
              RGT    B 110-86-1 Pyridine  
              PRO    AS 223590-62-3  
              NTE    4 H

RX(67) OF 106 COMPOSED OF RX(7), RX(29)  
 RX(67)      Q + C + AC ==> AT

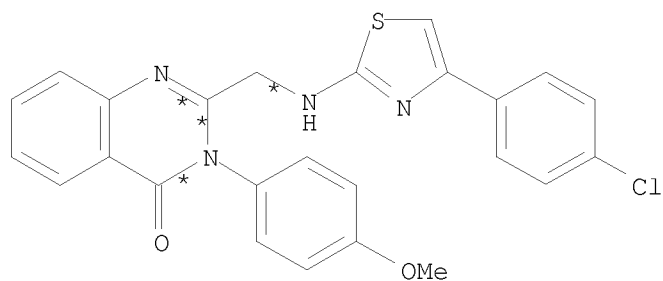


C



AC

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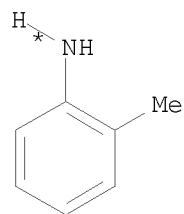


AT  
YIELD 62%

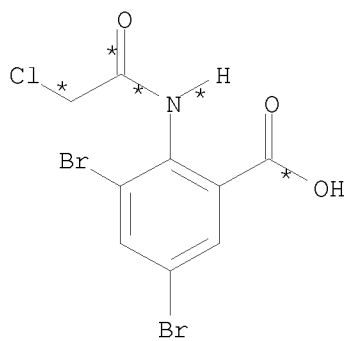
RX(7)        RCT    Q 104-94-9, C 14422-49-2  
              RGT    I 584-08-7 K2CO3  
              PRO    R 22312-82-9  
              SOL    64-17-5 EtOH  
              NTE    6 H

RX(29)       RCT    AC 2103-99-3, R 22312-82-9  
              RGT    B 110-86-1 Pyridine  
              PRO    AT 223590-63-4  
              NTE    4 H

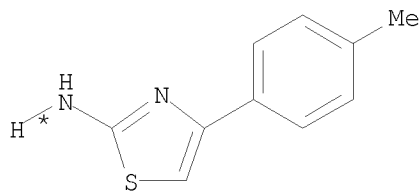
RX(68) OF 106 COMPOSED OF RX(8), RX(32)  
RX(68)       G   +   F   +   Z   ==>   AX



G



F

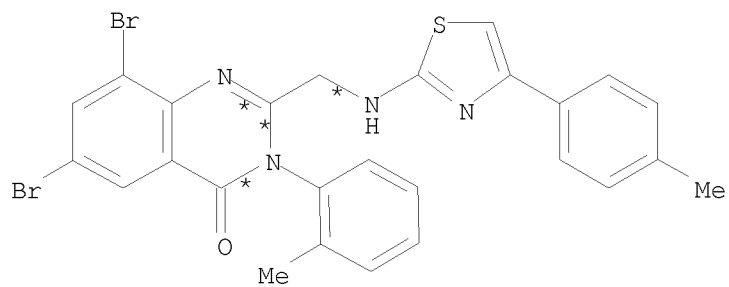


Z

2  
STEPS  
→



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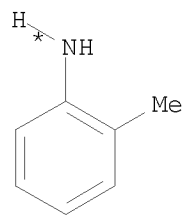


AX  
YIELD 54%

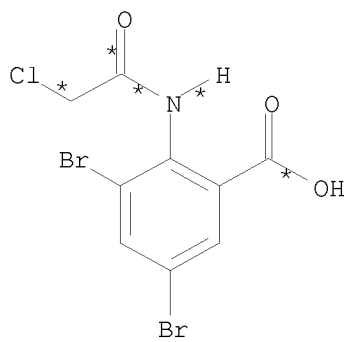
RX(8)      RCT    G 95-53-4, F 103952-88-1  
              RGT    I 584-08-7 K2CO3  
              PRO    S 177167-07-6  
              SOL    64-17-5 EtOH  
              NTE    6 H

RX(32)      RCT    Z 2103-91-5, S 177167-07-6  
              RGT    B 110-86-1 Pyridine  
              PRO    AX 223590-66-7  
              NTE    4 H

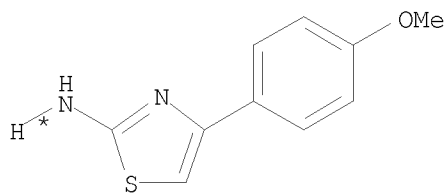
RX(69) OF 106 COMPOSED OF RX(8), RX(33)  
RX(69)      G    +    F    +    AG    ==>    AY



G



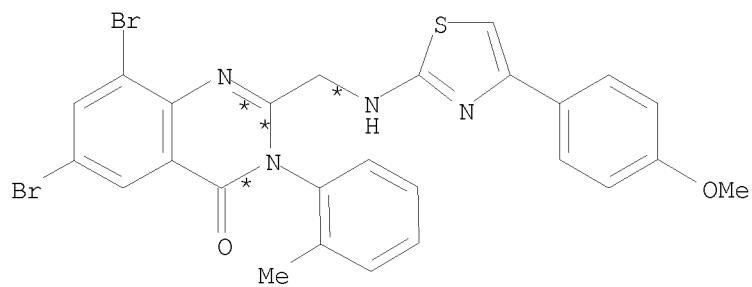
F



AG

2  
STEPS  
→

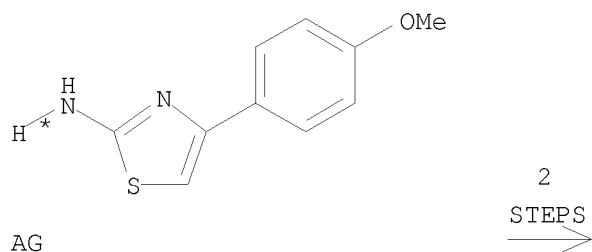
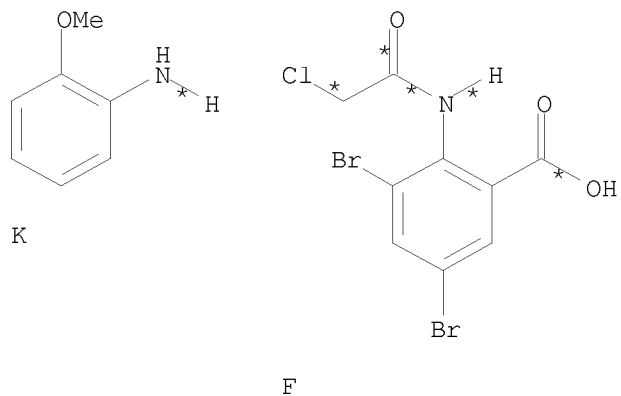
10/ 562,112



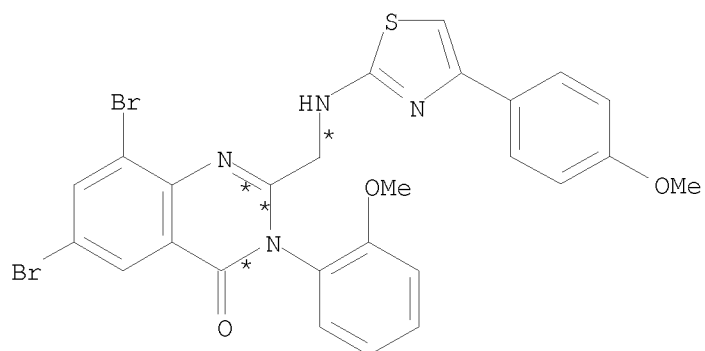
AY  
YIELD 54%

RX(8)	RCT	G 95-53-4, F 103952-88-1
	RGT	I 584-08-7 K2CO3
	PRO	S 177167-07-6
	SOL	64-17-5 EtOH
	NTE	6 H
RX(33)	RCT	AG 2104-04-3, S 177167-07-6
	RGT	B 110-86-1 Pyridine
	PRO	AY 223590-67-8
	NTE	4 H

RX(70) OF 106 COMPOSED OF RX(9), RX(34)  
RX(70) K + F + AG ==> AZ



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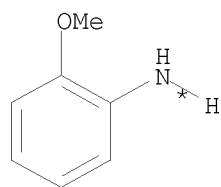


AZ  
YIELD 56%

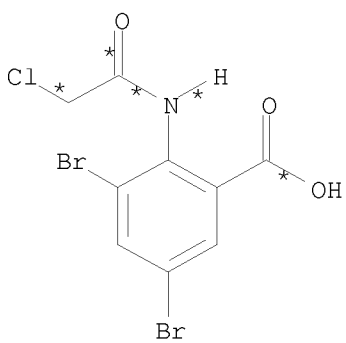
RX(9)      RCT    K 90-04-0, F 103952-88-1  
             RGT    I 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
             PRO    T 104308-99-8  
             SOL    64-17-5 EtOH  
             NTE    6 H

RX(34)      RCT    AG 2104-04-3, T 104308-99-8  
             RGT    B 110-86-1 Pyridine  
             PRO    AZ 223590-68-9  
             NTE    4 H

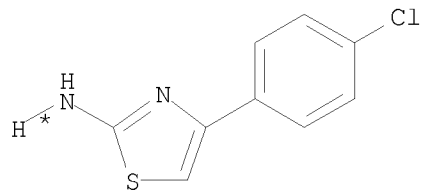
RX(71) OF 106 COMPOSED OF RX(9), RX(35)  
RX(71)      K + F + AC ==> BA



K



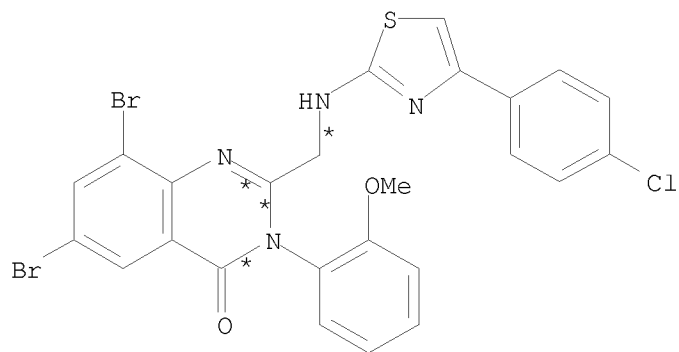
F



AC

2  
STEPS  
→

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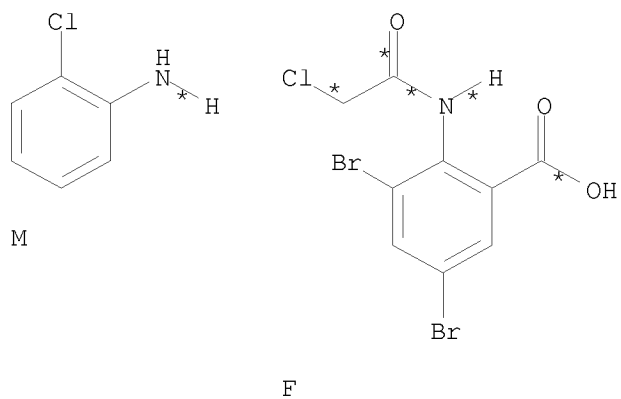


BA  
YIELD 57%

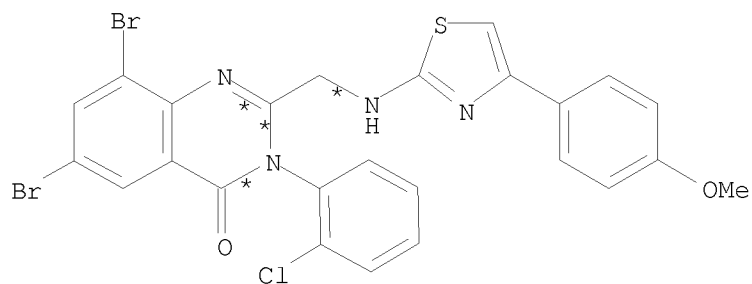
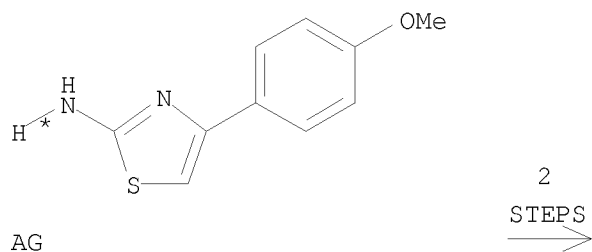
RX(9) RCT K 90-04-0, F 103952-88-1  
RGT I 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO T 104308-99-8  
SOL 64-17-5 EtOH  
NTE 6 H

RX(35) RCT AC 2103-99-3, T 104308-99-8  
RGT B 110-86-1 Pyridine  
PRO BA 223590-69-0  
NTE 4 H

RX(72) OF 106 COMPOSED OF RX(10), RX(36)  
RX(72) M + F + AG ==> BB



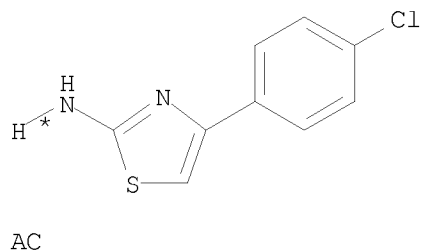
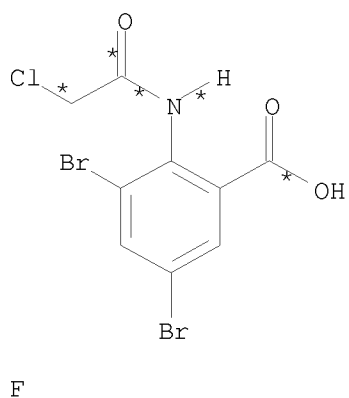
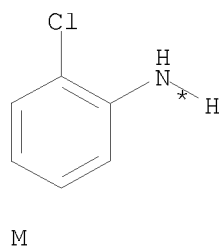
10/ 562,112



RX(10) RCT M 95-51-2, F 103952-88-1  
RGT I 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO U 104308-98-7  
SOL 64-17-5 EtOH  
NTE 6 H

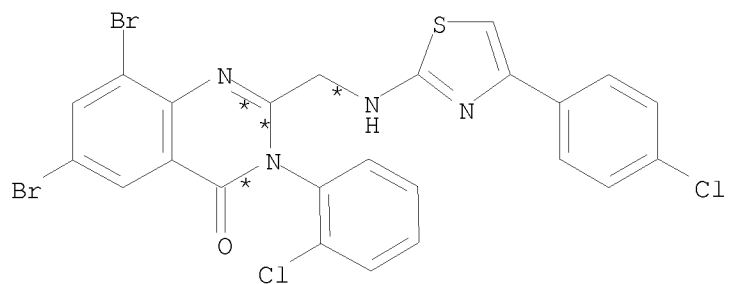
RX(36) RCT AG 2104-04-3, U 104308-98-7  
RGT B 110-86-1 Pyridine  
PRO BB 223590-70-3  
NTE 4 H

RX(73) OF 106 COMPOSED OF RX(10), RX(37)  
RX(73) M + F + AC ==> BC



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2  
STEPS  
→

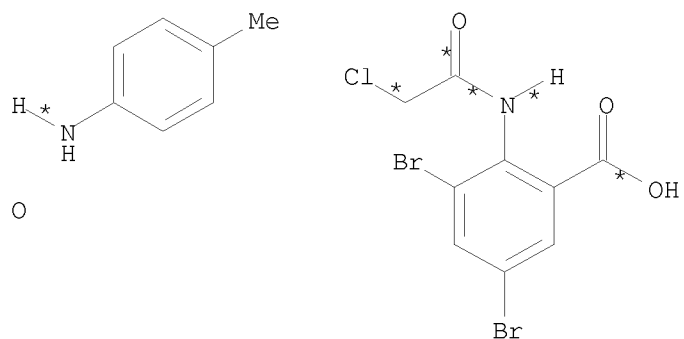


BC  
YIELD 51%

RX(10) RCT M 95-51-2, F 103952-88-1  
RGT I 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO U 104308-98-7  
SOL 64-17-5 EtOH  
NTE 6 H

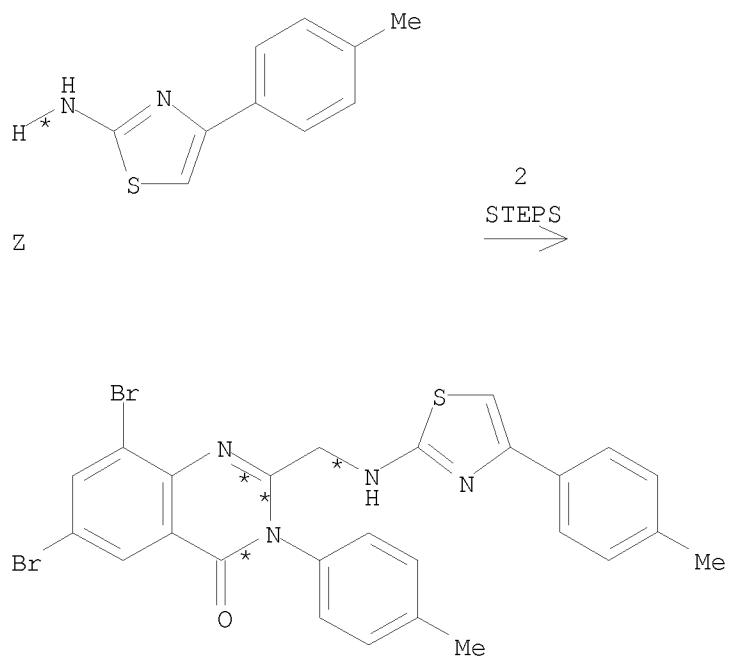
RX(37) RCT AC 2103-99-3, U 104308-98-7  
RGT B 110-86-1 Pyridine  
PRO BC 223590-71-4  
NTE 4 H

RX(74) OF 106 COMPOSED OF RX(11), RX(38)  
RX(74) O + F + Z ==> BD



F

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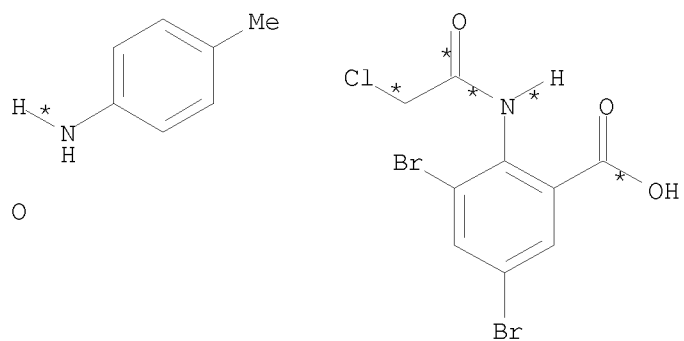


BD  
YIELD 59%

RX(11) RCT O 106-49-0, F 103952-88-1  
RGT I 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO V 103952-89-2  
SOL 64-17-5 EtOH  
NTE 6 H

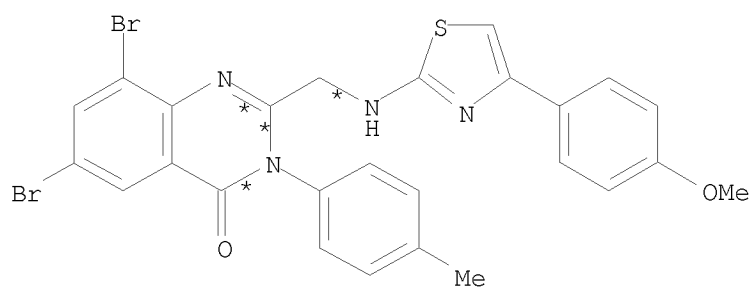
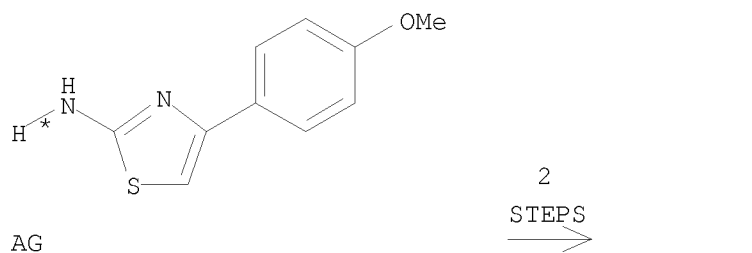
RX(38) RCT Z 2103-91-5, V 103952-89-2  
RGT B 110-86-1 Pyridine  
PRO BD 223590-72-5  
NTE 4 H

RX(75) OF 106 COMPOSED OF RX(11), RX(39)  
RX(75) O + F + AG ==> BE



F

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BE  
YIELD 49%

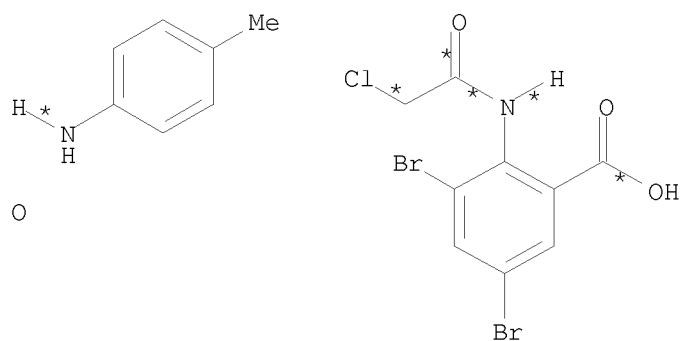
RX(11) RCT O 106-49-0, F 103952-88-1  
RGT I 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO V 103952-89-2  
SOL 64-17-5 EtOH  
NTE 6 H

RX(39) RCT AG 2104-04-3, V 103952-89-2  
RGT B 110-86-1 Pyridine  
PRO BE 223590-73-6  
NTE 4 H

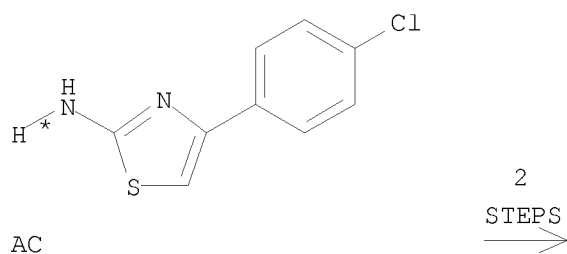
RX(76) OF 106 COMPOSED OF RX(11), RX(40)  
RX(76) O + F + AC ==> BF



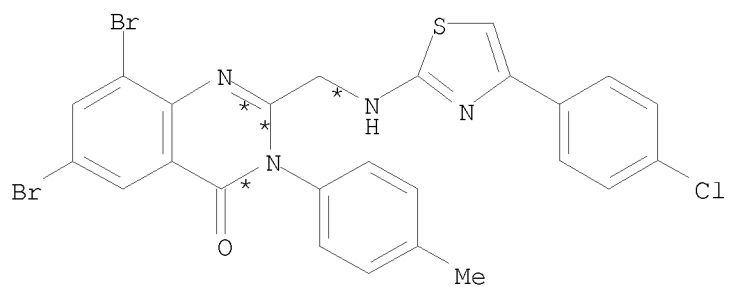
10/ 562,112



F



AC



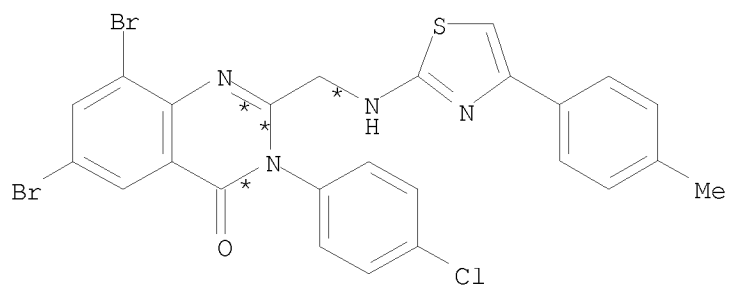
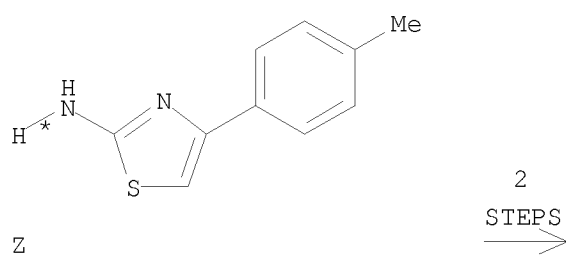
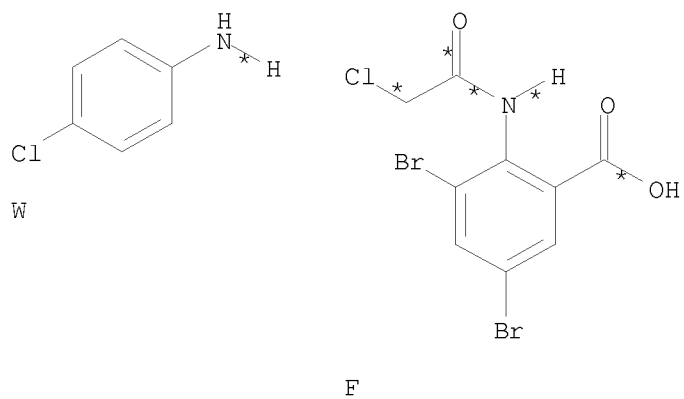
BF  
YIELD 60%

RX(11) RCT O 106-49-0, F 103952-88-1  
RGT I 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO V 103952-89-2  
SOL 64-17-5 EtOH  
NTE 6 H

RX(40) RCT AC 2103-99-3, V 103952-89-2  
RGT B 110-86-1 Pyridine  
PRO BF 223590-74-7  
NTE 4 H

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RX(77) OF 106 COMPOSED OF RX(12), RX(41)  
RX(77) W + F + Z ==> BG



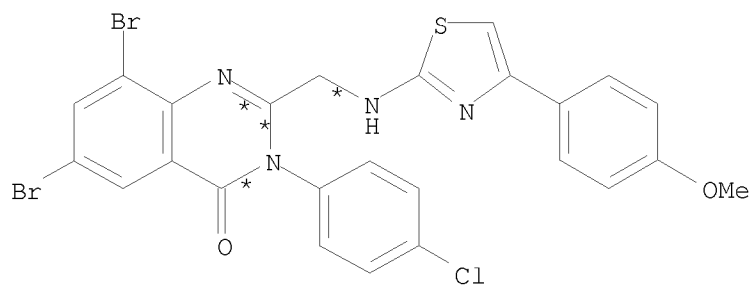
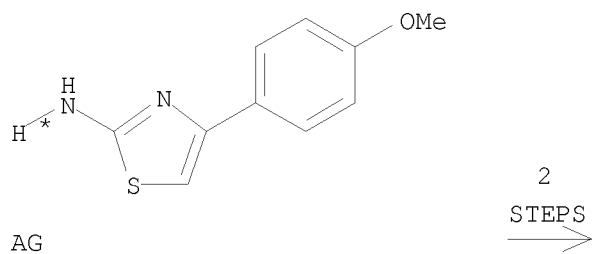
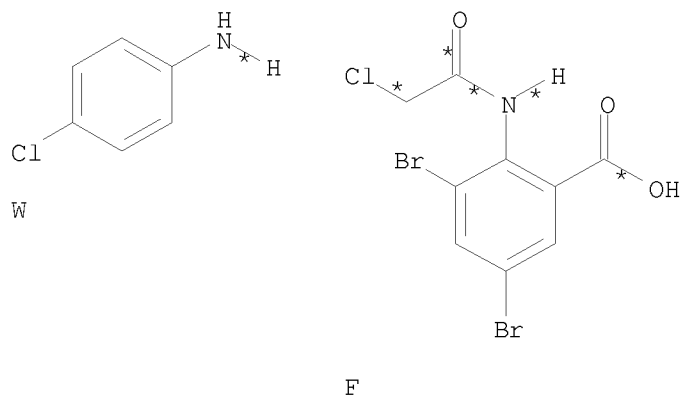
BG  
YIELD 47%

RX(12) RCT W 106-47-8, F 103952-88-1  
RGT I 584-08-7 K2CO3  
PRO X 223590-80-5  
SOL 64-17-5 EtOH  
NTE 6 H

RX(41) RCT Z 2103-91-5, X 223590-80-5  
RGT B 110-86-1 Pyridine  
PRO BG 223590-75-8  
NTE 4 H

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RX(78) OF 106 COMPOSED OF RX(12), RX(42)  
RX(78) W + F + AG ==> BH



BH  
YIELD 56%

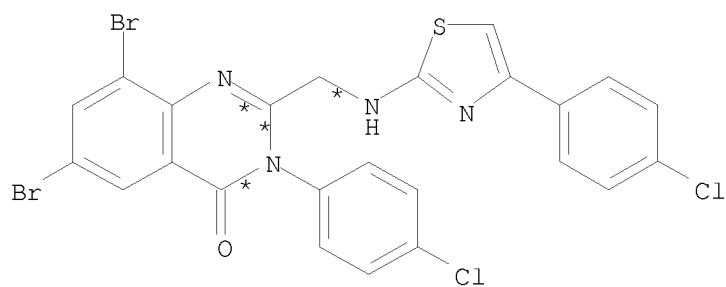
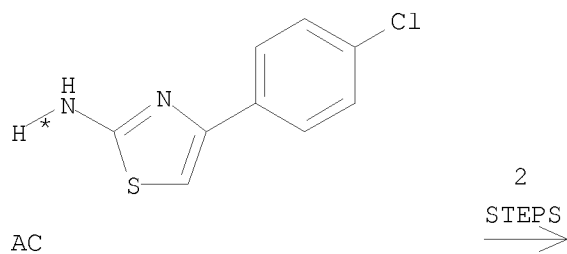
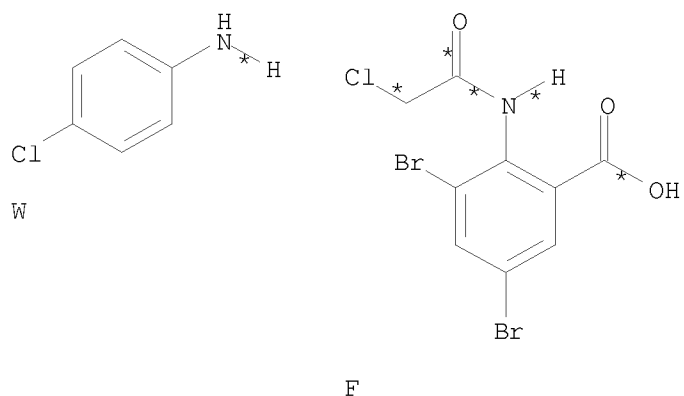
RX(12) RCT W 106-47-8, F 103952-88-1  
RGT I 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO X 223590-80-5  
SOL 64-17-5 EtOH  
NTE 6 H

RX(42) RCT AG 2104-04-3, X 223590-80-5  
RGT B 110-86-1 Pyridine

10/ 562,112

PRO BH 223590-76-9  
NTE 4 H

RX(79) OF 106 COMPOSED OF RX(12), RX(43)  
RX(79) W + F + AC ==> BI



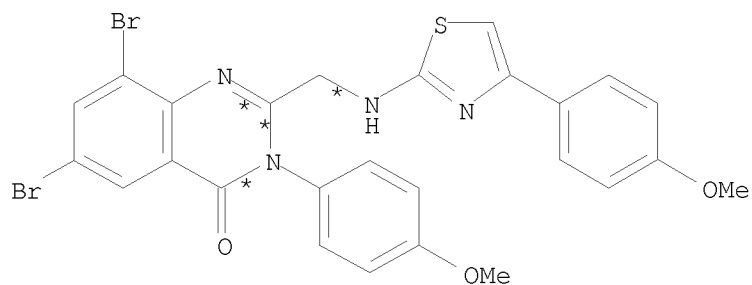
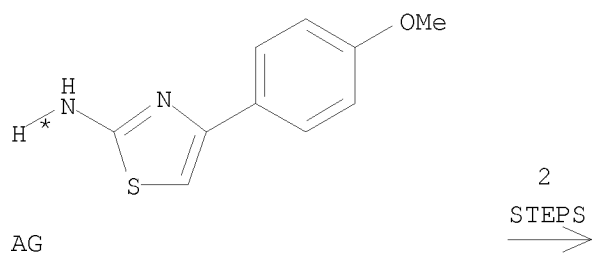
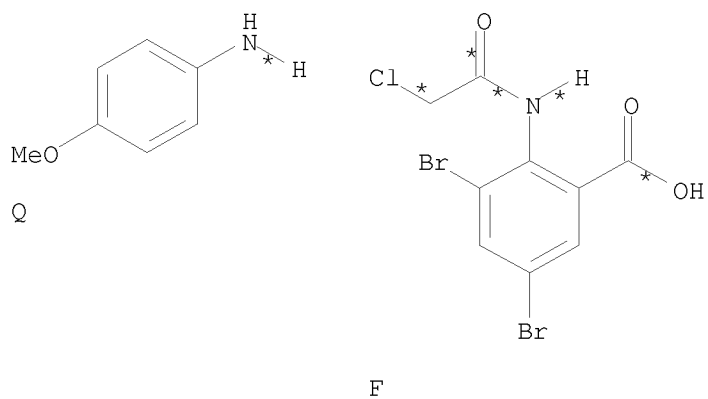
BI  
YIELD 59%

RX(12) RCT W 106-47-8, F 103952-88-1  
RGT I 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
PRO X 223590-80-5  
SOL 64-17-5 EtOH  
NTE 6 H

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RX(43) RCT AC 2103-99-3, X 223590-80-5  
RGT B 110-86-1 Pyridine  
PRO BI 223590-77-0  
NTE 4 H

RX(80) OF 106 COMPOSED OF RX(13), RX(44)  
RX(80) Q + F + AG ==> BJ



BJ  
YIELD 53%

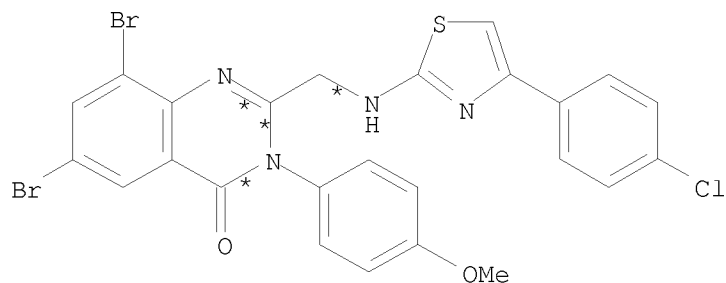
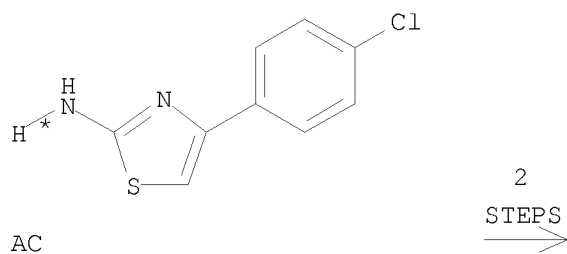
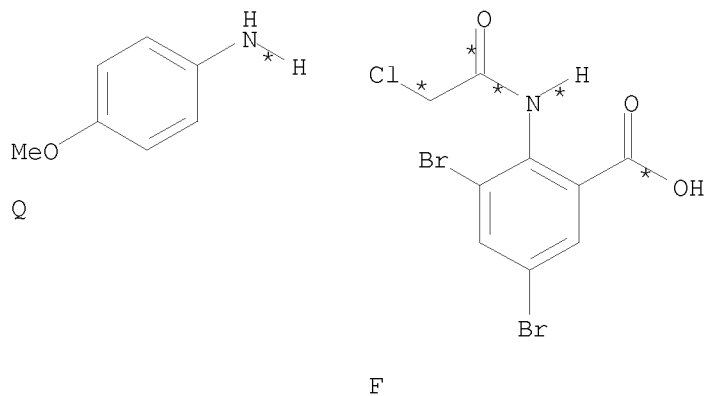
RX(13) RCT Q 104-94-9, F 103952-88-1  
RGT I 584-08-7 K2CO3  
PRO Y 223590-81-6  
SOL 64-17-5 EtOH

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NTE 6 H

RX(44) RCT AG 2104-04-3, Y 223590-81-6  
RGT B 110-86-1 Pyridine  
PRO BJ 223590-78-1  
NTE 4 H

RX(81) OF 106 COMPOSED OF RX(13), RX(45)  
RX(81) Q + F + AC ==> BK



BK  
YIELD 51%

RX(13) RCT Q 104-94-9, F 103952-88-1  
RGT I 584-08-7 K2CO3

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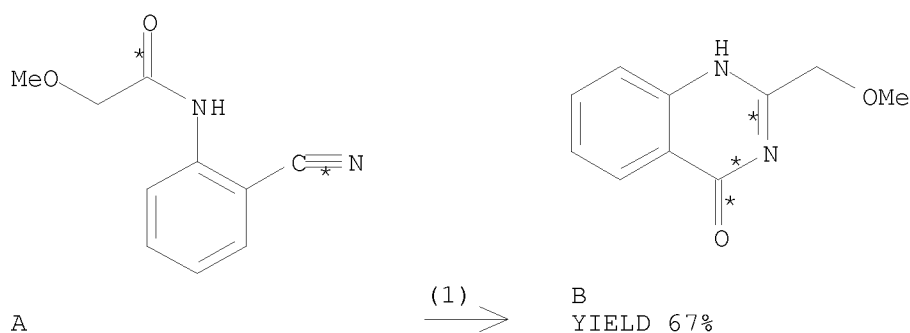
PRO Y 223590-81-6  
SOL 64-17-5 EtOH  
NTE 6 H

RX(45) RCT AC 2103-99-3, Y 223590-81-6  
RGT B 110-86-1 Pyridine  
PRO BK 223590-79-2  
NTE 4 H

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 120 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 130:110232 CASREACT  
TITLE: A facile route to quinazolin-4(3H)-ones functionalized  
at the 2-position  
AUTHOR(S): Bavetsias, V.  
CORPORATE SOURCE: CRC Laboratory, CRC Centre for Cancer Therapeutics at  
The Institute of Cancer Research, Surrey, SM2 5NG, UK  
SOURCE: Synthetic Communications (1998), 28(24), 4547-4559  
CODEN: SYNCAV; ISSN: 0039-7911  
PUBLISHER: Marcel Dekker, Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Treatment of 2-methoxyacetamidobenzonitriles or  
2-chloroacetamidobenzonitrile with UHP and K<sub>2</sub>CO<sub>3</sub> provides a convenient  
route to 2-methoxymethyl- or 2-chloromethylquinazolin-4(3H)-ones. In  
addition, demethylation of 2-methoxymethylquinazolin-4(3H)-ones with 48% HBr  
gives 2-hydroxymethylquinazolin-4(3H)-ones.

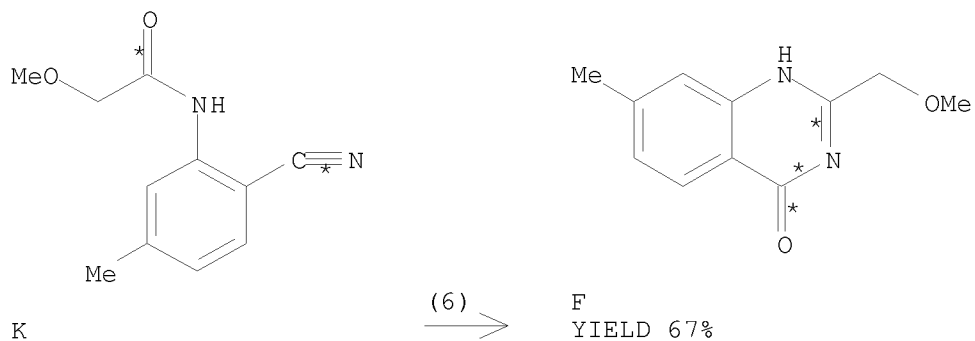
RX(1) OF 12 A ==> B...



RX(1) RCT A 219739-45-4  
PRO B 21721-76-6  
SOL 67-64-1 Me<sub>2</sub>CO  
NTE 50 H, 82.deg.

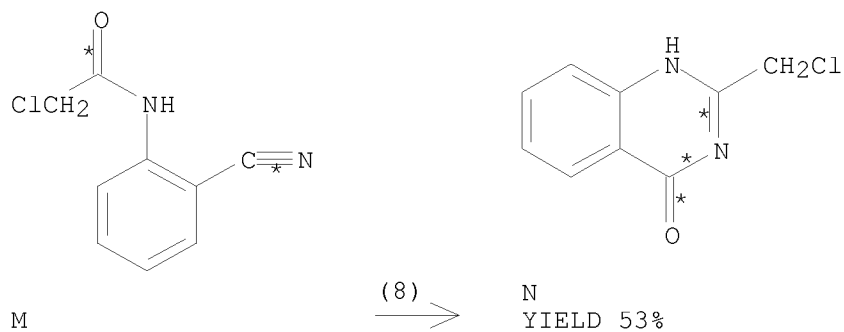
RX(6) OF 12 K ==> F...

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RX(6) RCT K 219739-46-5  
PRO F 219739-48-7  
SOL 67-64-1 Me2CO  
NTE 46 H, 82.deg.

RX(8) OF 12 M ==> N

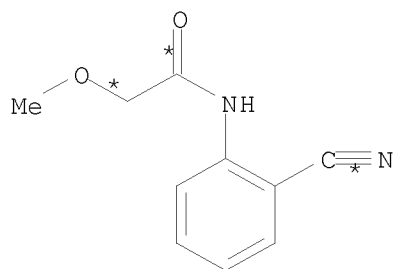


RX(8) RCT M 71993-21-0  
PRO N 3817-05-8  
SOL 67-64-1 Me2CO  
NTE 30 H, 84.deg.

RX(9) OF 12 COMPOSED OF RX(1), RX(2)  
RX(9) A ==> D

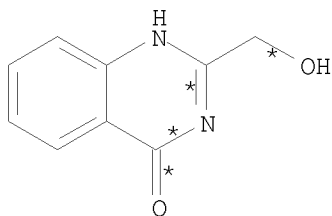


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A

2  
STEPS  
→

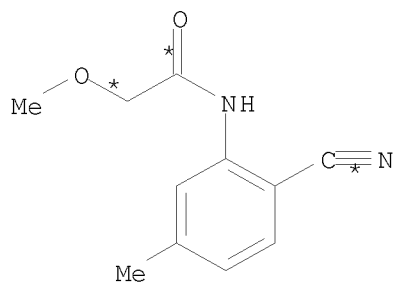


D  
YIELD 61%

RX(1) RCT A 219739-45-4  
PRO B 21721-76-6  
SOL 67-64-1 Me2CO  
NTE 50 H, 82.deg.

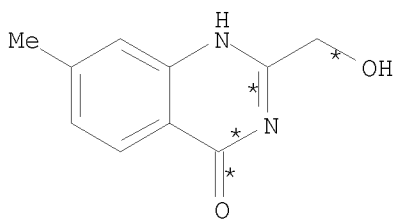
RX(2) RCT B 21721-76-6  
RGT E 10035-10-6 HBr  
PRO D 34637-40-6  
NTE 11 H, 120.deg.

RX(10) OF 12 COMPOSED OF RX(6), RX(3)  
RX(10) K ==> G



K

2  
STEPS  
→

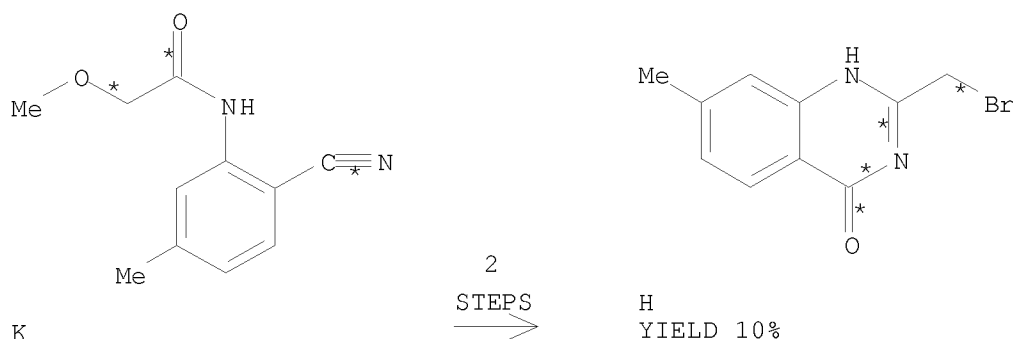


G  
YIELD 61%

RX(6) RCT K 219739-46-5  
PRO F 219739-48-7  
SOL 67-64-1 Me2CO  
NTE 46 H, 82.deg.

RX(3) RCT F 219739-48-7  
RGT E 10035-10-6 HBr  
PRO G 219739-50-1  
NTE 6 H, 120.deg.

RX(11) OF 12 COMPOSED OF RX(6), RX(4)  
RX(11) K ==> H



RX(6) RCT K 219739-46-5  
 PRO F 219739-48-7  
 SOL 67-64-1 Me2CO  
 NTE 46 H, 82.deg.

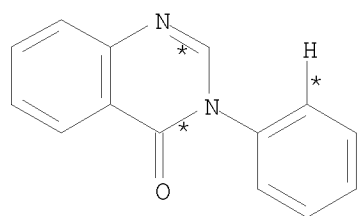
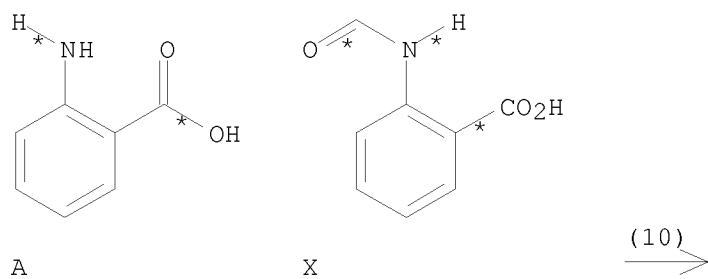
RX(4) RCT F 219739-48-7  
 RGT E 10035-10-6 HBr  
 PRO H 219739-51-2  
 NTE 6 H, 120.deg.

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 121 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 130:81480 CASREACT  
 TITLE: One-pot synthesis of substituted quinazolin-4(3H)-ones under microwave irradiation  
 AUTHOR(S): Rad-Moghadam, Kurosh; Khajavi, Mohammad S.  
 CORPORATE SOURCE: Chemistry Department, Shahid Beheshti University, Tehran, 19839, Iran  
 SOURCE: Journal of Chemical Research, Synopses (1998), (11), 702-703  
 CODEN: JRPSDC; ISSN: 0308-2342  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Synthesis of the title compds. by cyclocondensation of anthranilic acid, formic acid (or an ortho ester) and an amine in one pot under microwave irradiation takes place in a few minutes.

RX(10) OF 11 A + X ==> J

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J  
YIELD 71%

RX(10) RCT A 118-92-3, X 3342-77-6

STAGE(1)

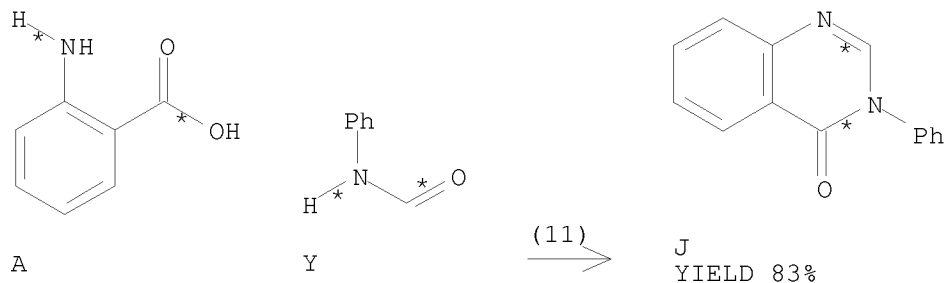
STAGE(2)

SOL 7732-18-5 Water, 64-17-5 EtOH

PRO J 16347-60-7

NTE microwave irradiation without solvent in first stage

RX(11) OF 11 A + Y ==> J



RX(11) RCT A 118-92-3, Y 103-70-8

STAGE(1)

RGT Z 127-19-5 AcNMe2

STAGE(2)

SOL 7732-18-5 Water, 64-17-5 EtOH

PRO J 16347-60-7

NTE microwave irradiation without solvent in first stage

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 122 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 129:343135 CASREACT

TITLE: Diastereoselective aziridination of alkenes using  
3-acetoxymino-2-(1-hydroxyalkyl)quinazolin-4(3H)-ones  
in the presence of titanium(IV) tert-butoxide

AUTHOR(S): Atkinson, Robert S.; Ayscough, Andrew P.; Gattrell, W.  
T.; Raynham, Tony M.

CORPORATE SOURCE: Dep. Chem., Univ. Leicester, LE1 7RH, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions  
1: Organic and Bio-Organic Chemistry (1998), (17),  
2783-2793

CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER: Royal Society of Chemistry

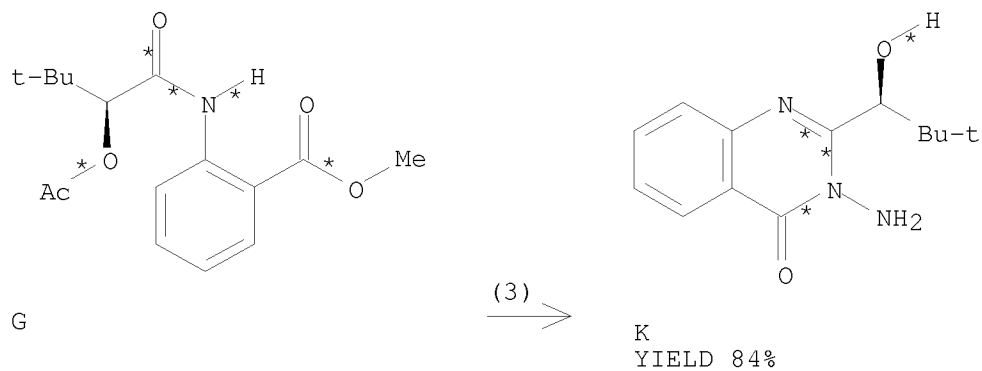
DOCUMENT TYPE: Journal

LANGUAGE: English

AB 3-Amino-2-[(S)-1-hydroxy-2,2-dimethylpropyl]quinazolin-4(3H)-one 9 (Q2NH) was prepared in four steps from (S)-tert-leucine in 43% yield without the need for chromatography. The corresponding 3-acetoxyminoquinazolinone, prepared in dichloromethane solution by reaction of 9 with lead tetraacetate, reacts with alkenes in the presence of titanium(IV) tert-butoxide to give the corresponding aziridines stereoselectively. With styrene and butadiene the corresponding aziridines were obtained completely stereoselectively. Indene gave the expected endo-N-invertomer of aziridine as the kinetically-formed product (86%) also completely stereoselectively; equilibration to give a 8:1 ratio of exo:endo N-invertomers occurs above 0°C. From an X-ray structure determination one aziridine product, the sense of diastereoselectivity in its formation is in agreement with the transition state model. Aziridinations of Me acrylate and of tert-Bu acrylate give the resp. products highly stereoselectively (dr ≥ 20:1) and with the same sense of diastereoselectivity as identified by an X-ray crystal structure determination previously. Aziridinations of  $\alpha$ -methylstyrene and Me methacrylate are less completely diastereoselective; isoprene reacts completely diastereoselectively at its unsubstituted double bond but with little diastereoselectivity at its methyl-substituted double bond and the regioselectivity of aziridination on the two double bonds is 1.4:1 resp. by comparison to 1:4.7 in the absence of titanium(IV) tert-butoxide.

RX(3) OF 127 ...G ==&gt; K...

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RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

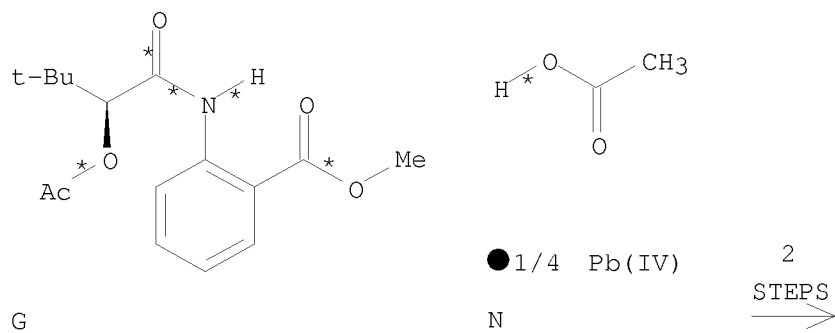
SOL 7732-18-5 Water

PRO K 182160-10-7

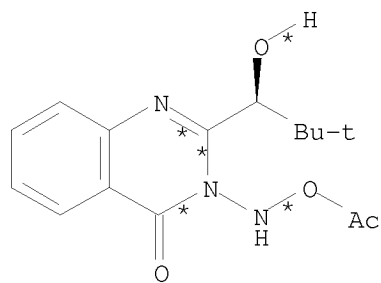
NTE STEREOSELECTIVE

RX(28) OF 127 COMPOSED OF RX(3), RX(4)

RX(28) G + N ==> O



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O

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4  
SOL 64-17-5 EtOH

STAGE(2)

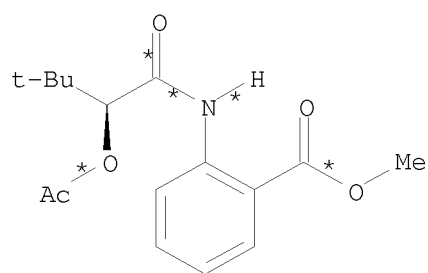
SOL 7732-18-5 Water

PRO K 182160-10-7  
NTE STEREOSELECTIVE

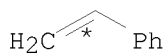
RX(4) RCT K 182160-10-7, N 546-67-8  
PRO O 182160-08-3  
SOL 865-49-6 CDCl3  
NTE STEREOSELECTIVE

RX(29) OF 127 COMPOSED OF RX(3), RX(5)

RX(29) 2 G + 2 Q ==> R + S



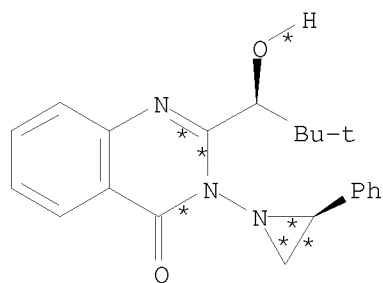
2 G



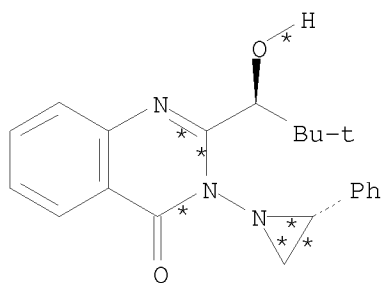
2 Q

2  
STEPS  
→

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R  
YIELD 90%(40)



S  
YIELD 90%(60)

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(5) RCT K 182160-10-7

STAGE(1)

RGT N 546-67-8 Pb(OAc)4

STAGE(2)

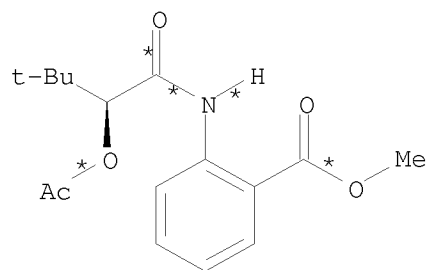
RCT Q 100-42-5

PRO R 182160-14-1, S 182267-16-9

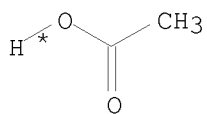
NTE STEREOSELECTIVE

RX(57) OF 127 COMPOSED OF RX(3), RX(4), RX(6)

RX(57) 2 G + 2 N + T + Q ==> R + U

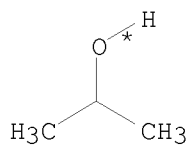


2 G



● 1/4 Pb(IV)

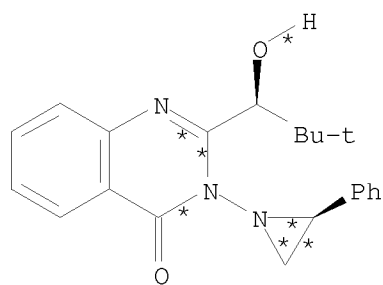
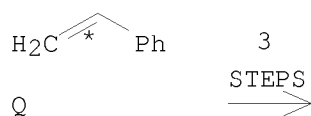
2 N



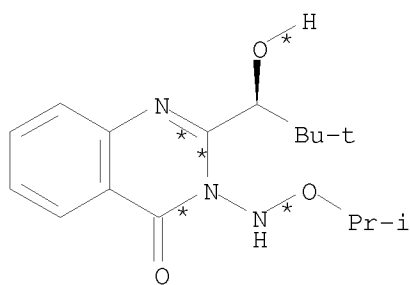
● 1/4 Ti(IV)

T

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R  
YIELD 14%



U  
YIELD 59%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDCl3

NTE STEREOSELECTIVE

RX(6) RCT O 182160-08-3, T 546-68-9, Q 100-42-5

PRO R 182160-14-1, U 215546-93-3

SOL 75-09-2 CH2Cl2

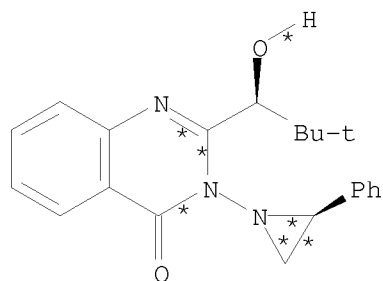
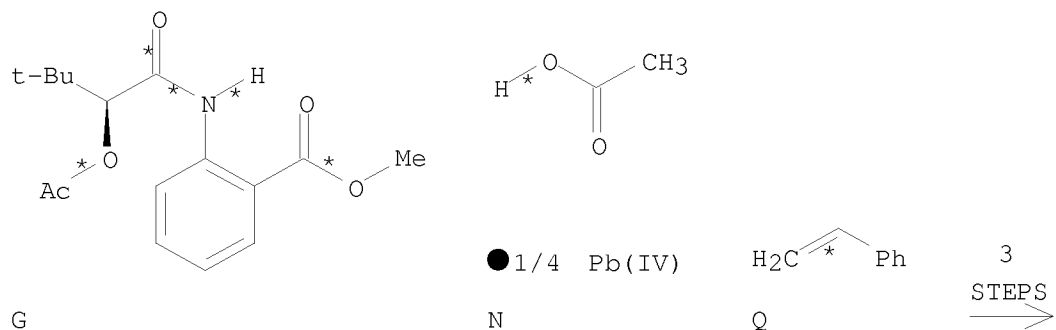
NTE STEREOSELECTIVE

RX(58) OF 127 COMPOSED OF RX(3), RX(4), RX(7)

RX(58) G + N + Q ==> R



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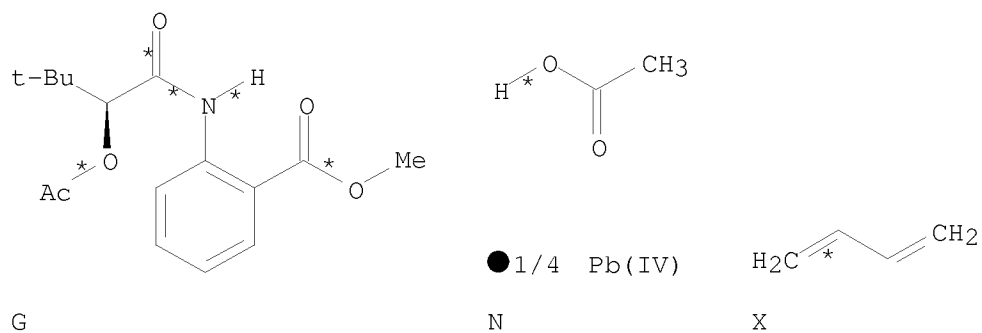


R  
YIELD 65%

RX(3) RCT G 215546-92-2  
 STAGE(1)  
 RGT L 302-01-2 N2H4  
 SOL 64-17-5 EtOH  
 STAGE(2)  
 SOL 7732-18-5 Water  
 PRO K 182160-10-7  
 NTE STEREOSELECTIVE  
 RX(4) RCT K 182160-10-7, N 546-67-8  
 PRO O 182160-08-3  
 SOL 865-49-6 CDCl3  
 NTE STEREOSELECTIVE  
 RX(7) RCT O 182160-08-3, Q 100-42-5  
 RGT W 3087-39-6 (t-BuO)4Ti  
 PRO R 182160-14-1  
 SOL 75-09-2 CH2Cl2  
 NTE STEREOSELECTIVE

RX(59) OF 127 COMPOSED OF RX(3), RX(4), RX(8)  
 RX(59) G + N + X ==> Y

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RX(3) RCT G 215546-92-2

STAGE(1)  
RGT L 302-01-2 N2H4  
SOL 64-17-5 EtOH

STAGE(2)  
SOL 7732-18-5 Water

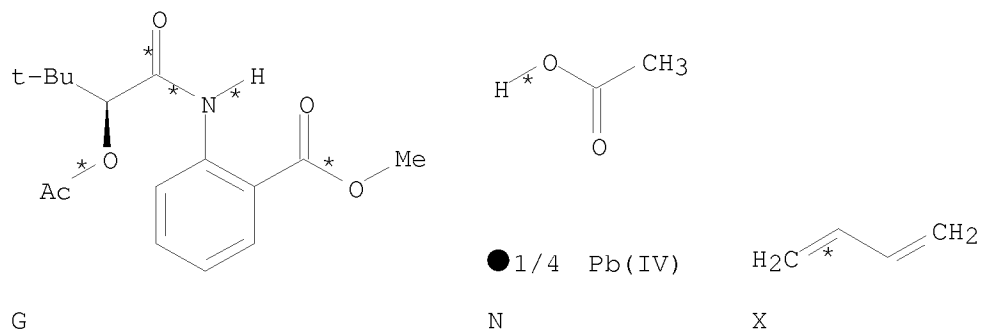
PRO K 182160-10-7  
NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8  
PRO O 182160-08-3  
SOL 865-49-6 CDC13  
NTE STEREOSELECTIVE

RX(8) RCT O 182160-08-3, X 106-99-0  
PRO Y 182267-17-0  
SOL 75-09-2 CH2Cl2  
NTE STEREOSELECTIVE

RX(60) OF 127 COMPOSED OF RX(3), RX(4), RX(9)  
RX(60) G + N + X ==> Z

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RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDCl3

NTE STEREOSELECTIVE

RX(9) RCT O 182160-08-3, X 106-99-0

RGT W 3087-39-6 (t-BuO)4Ti

PRO Z 182160-17-4

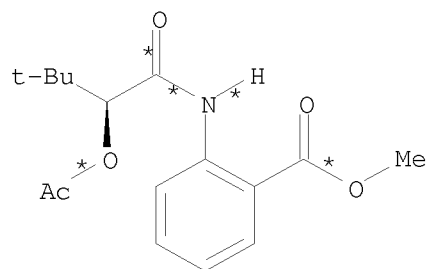
SOL 75-09-2 CH2Cl2

NTE STEREOSELECTIVE

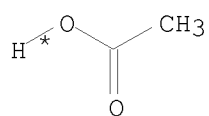
RX(61) OF 127 COMPOSED OF RX(3), RX(4), RX(10)

RX(61) G + N + AA ==> AB

10/ 562,112

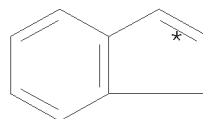


G



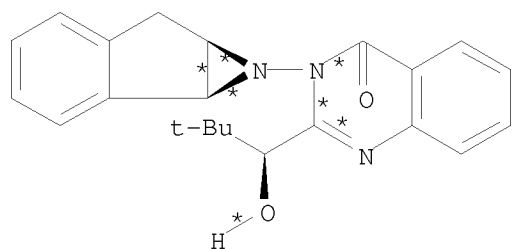
● 1/4 Pb(IV)

N



AA

3  
STEPS  
→



AB  
YIELD 86%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDCl3

NTE STEREOSELECTIVE

RX(10) RCT O 182160-08-3, AA 95-13-6

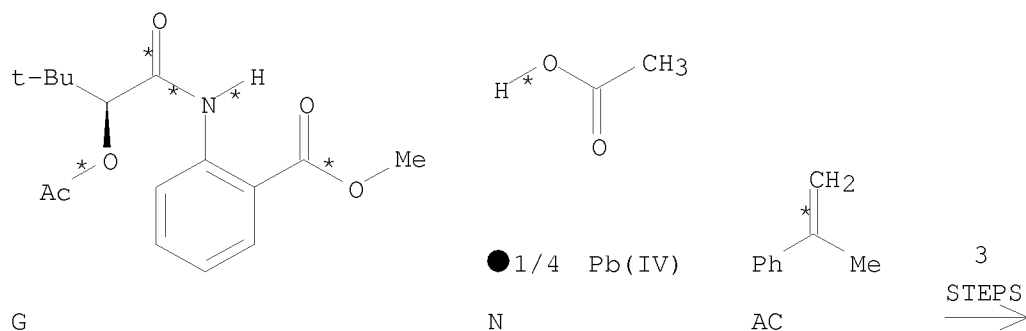
PRO AB 182267-18-1

SOL 75-09-2 CH2Cl2

NTE STEREOSELECTIVE

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RX(62) OF 127 COMPOSED OF RX(3), RX(4), RX(11)  
RX(62) G + N + AC ==> AD



AD  
YIELD 77%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4  
SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7  
NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8  
PRO O 182160-08-3  
SOL 865-49-6 CDCl3  
NTE STEREOSELECTIVE

RX(11) RCT O 182160-08-3, AC 98-83-9

STAGE(1)

SOL 75-09-2 CH2Cl2

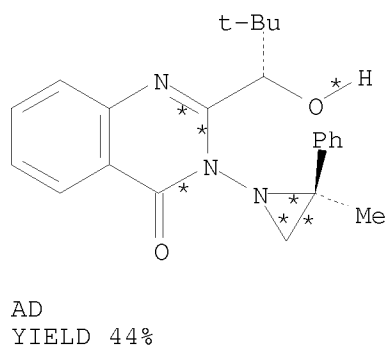
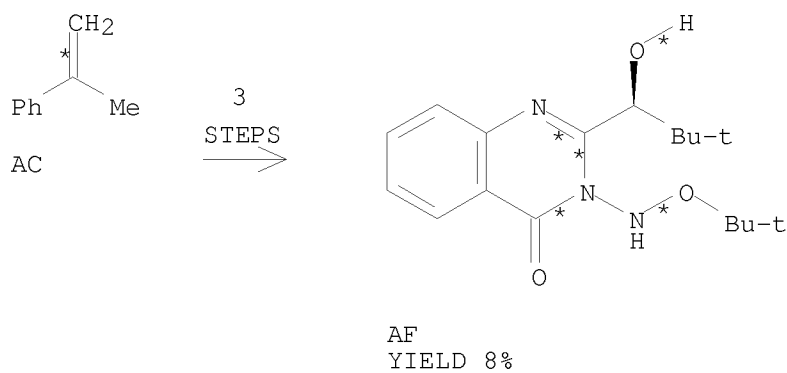
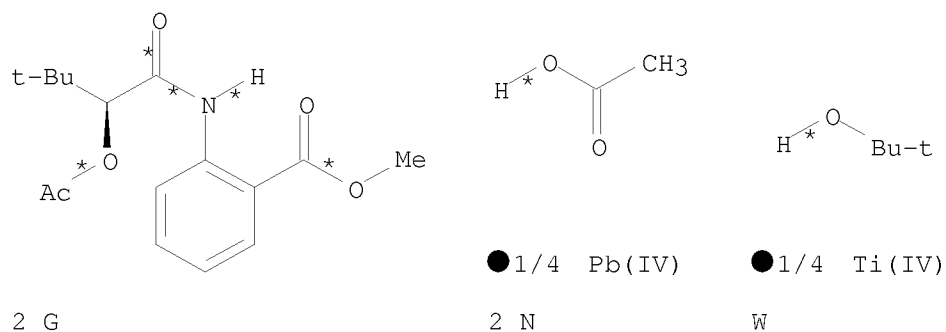
STAGE(2)

RGT AE 144-55-8 NaHCO3  
SOL 7732-18-5 Water

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PRO AD 215546-94-4  
NTE STEREOSELECTIVE

RX(63) OF 127 COMPOSED OF RX(3), RX(4), RX(12)  
RX(63) 2 G + 2 N + W + AC ==> AF + AD



RX(3) RCT G 215546-92-2

STAGE(1)  
RGT L 302-01-2 N2H4  
SOL 64-17-5 EtOH

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STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7  
NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8  
PRO O 182160-08-3  
SOL 865-49-6 CDC13  
NTE STEREOSELECTIVE

RX(12) RCT O 182160-08-3, W 3087-39-6, AC 98-83-9

STAGE(1)

SOL 75-09-2 CH2Cl2

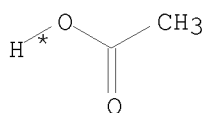
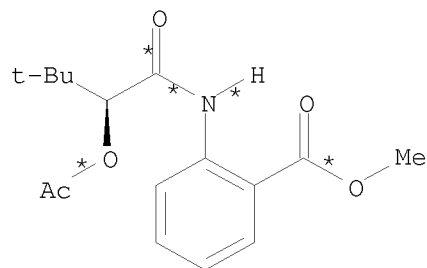
STAGE(2)

RGT AE 144-55-8 NaHCO3  
SOL 7732-18-5 Water

PRO AF 215546-95-5, AD 215546-94-4  
NTE STEREOSELECTIVE

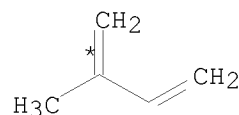
RX(64) OF 127 COMPOSED OF RX(3), RX(4), RX(13)

RX(64) 4 G + 4 N + 3 AG ==> AH + AI + AJ +  
AK

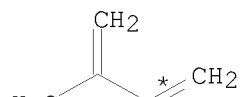


● 1/4 Pb(IV)

4 N

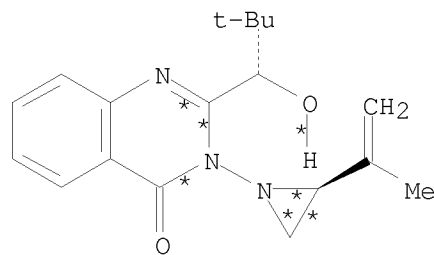


2 AG



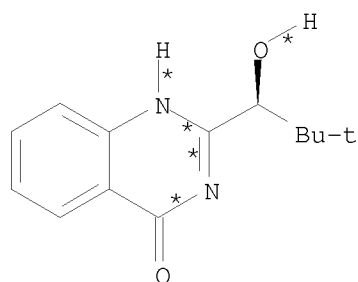
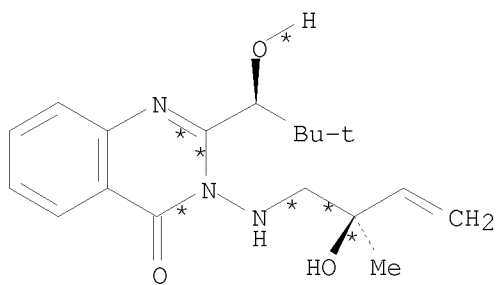
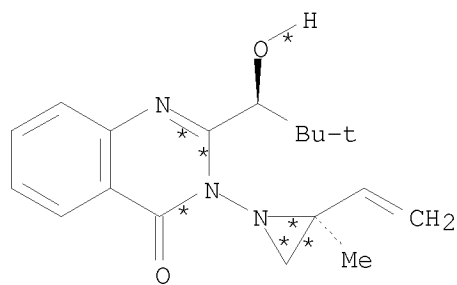
AG

3  
STEPS  
→



AH  
YIELD 10%

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RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDCl3

NTE STEREOSELECTIVE

RX(13) RCT O 182160-08-3, AG 78-79-5

PRO AH 215546-97-7, AI 215546-96-6, AJ 215546-98-8, AK  
215546-99-9

SOL 75-09-2 CH2Cl2

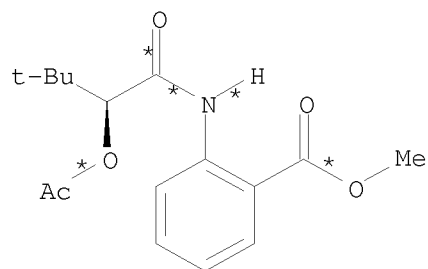
NTE STEREOSELECTIVE

RX(65) OF 127 COMPOSED OF RX(3), RX(4), RX(14)

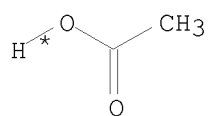
RX(65) 2 G + 2 N + 2 AG ==> AH + AI



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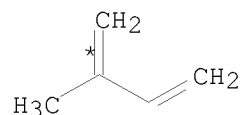


2 G

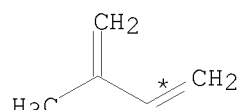


● 1/4 Pb(IV)

2 N

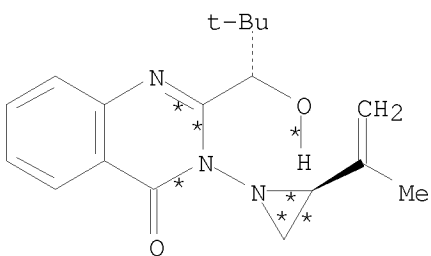


AG

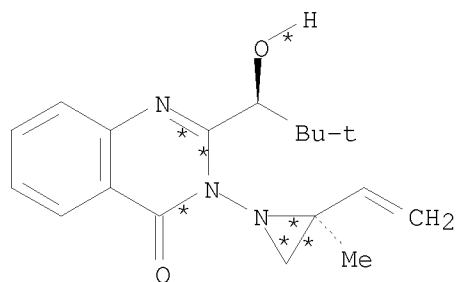


AG

3  
STEPS  
=>



AH  
YIELD 30%



AI  
YIELD 30%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

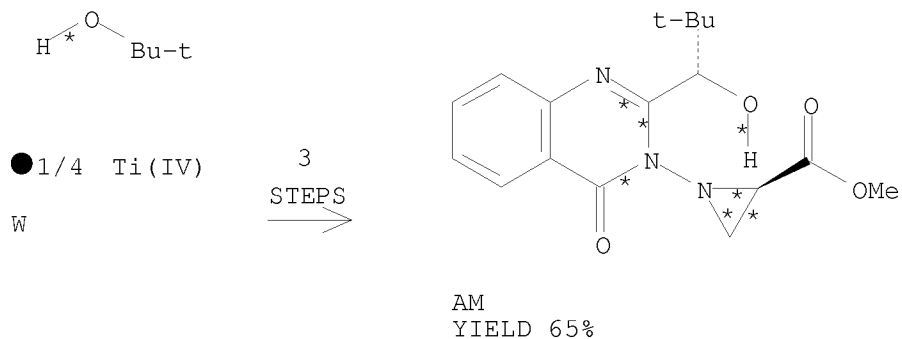
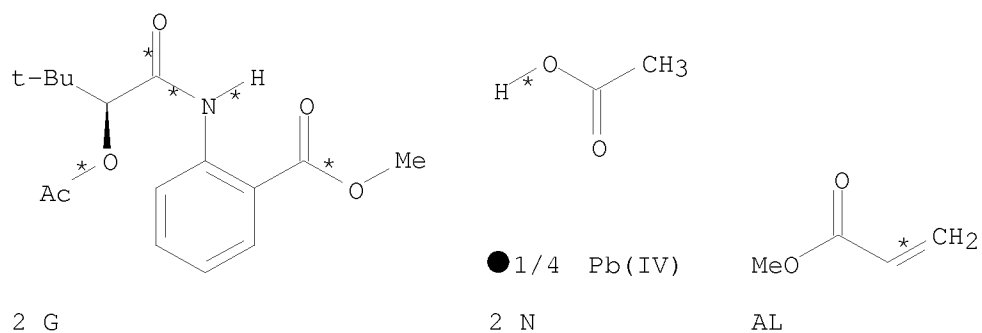
NTE STEREOSELECTIVE

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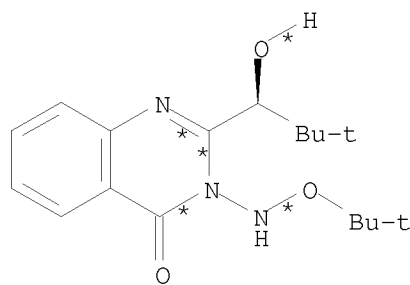
RX(4) RCT K 182160-10-7, N 546-67-8  
 PRO O 182160-08-3  
 SOL 865-49-6 CDC13  
 NTE STEREOSELECTIVE

RX(14) RCT O 182160-08-3, AG 78-79-5  
 RGT W 3087-39-6 (t-BuO)4Ti  
 PRO AH 215546-97-7, AI 215546-96-6  
 SOL 75-09-2 CH2Cl2  
 NTE STEREOSELECTIVE

RX(66) OF 127 COMPOSED OF RX(3), RX(4), RX(15)  
 RX(66) 2 G + 2 N + AL + W ==> AM + AF



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AF  
YIELD 25%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDCl3

NTE STEREOSELECTIVE

RX(15) RCT O 182160-08-3, AL 96-33-3, W 3087-39-6

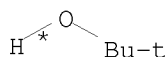
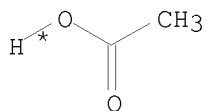
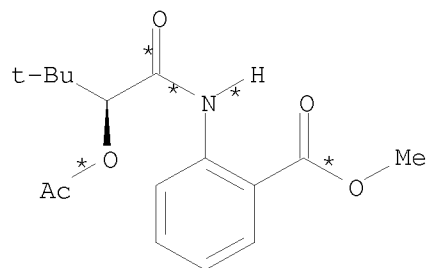
PRO AM 215547-00-5, AF 215546-95-5

SOL 75-09-2 CH2Cl2

NTE STEREOSELECTIVE

RX(67) OF 127 COMPOSED OF RX(3), RX(4), RX(16)

RX(67) G + N + AN ==> AF



● 1/4 Pb(IV)

● 1/4 Zr(IV)

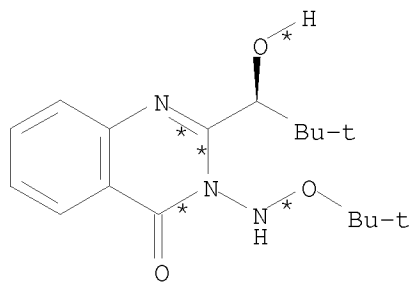
G

N

AN

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3  
STEPS  
→



AF  
YIELD 56%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDCl3

NTE STEREOSELECTIVE

RX(16) RCT O 182160-08-3, AN 2081-12-1

RGT AL 96-33-3 Me acrylate

PRO AF 215546-95-5

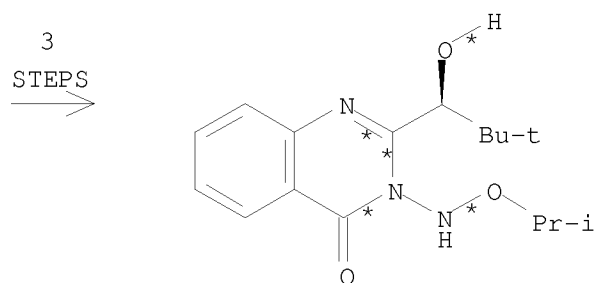
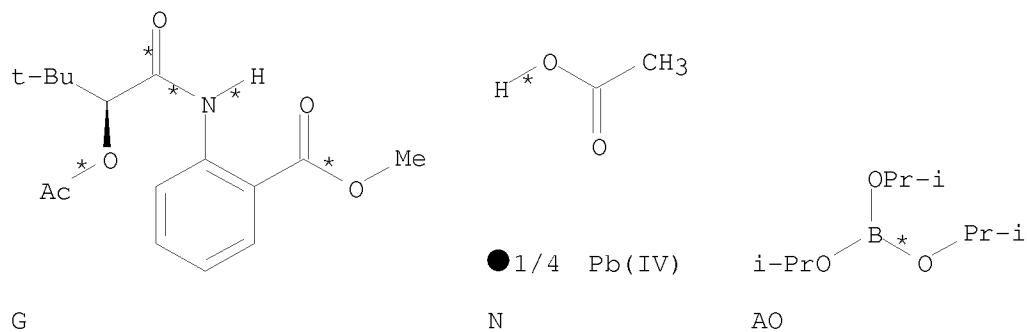
SOL 75-09-2 CH2Cl2

NTE STEREOSELECTIVE

RX(68) OF 127 COMPOSED OF RX(3), RX(4), RX(17)

RX(68) G + N + AO ==> U

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U  
YIELD 75%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N<sub>2</sub>H<sub>4</sub>  
SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

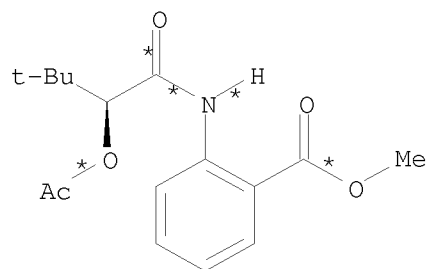
PRO K 182160-10-7  
NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8  
PRO O 182160-08-3  
SOL 865-49-6 CDCl<sub>3</sub>  
NTE STEREOSELECTIVE

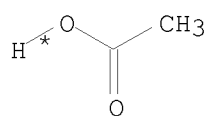
RX(17) RCT O 182160-08-3, AO 5419-55-6  
RGT AL 96-33-3 Me acrylate  
PRO U 215546-93-3  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
NTE STEREOSELECTIVE

RX(69) OF 127 COMPOSED OF RX(3), RX(4), RX(18)  
RX(69) 2 G + 2 N + 2 AL ==> AM + AP

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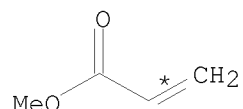


2 G



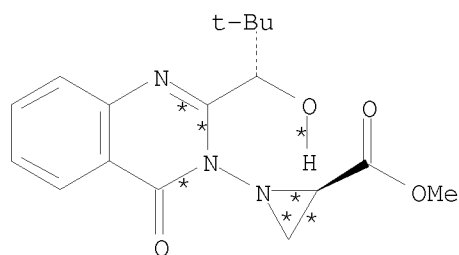
● 1/4 Pb(IV)

2 N

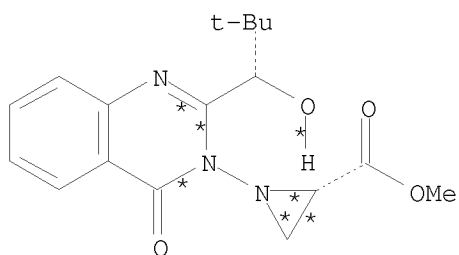


2 AL

3  
STEPS  
→



AM  
YIELD 74%(25)



AP  
YIELD 74%(75)

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDC13

NTE STEREOSELECTIVE

RX(18) RCT O 182160-08-3, AL 96-33-3

PRO AM 215547-00-5, AP 215547-01-6

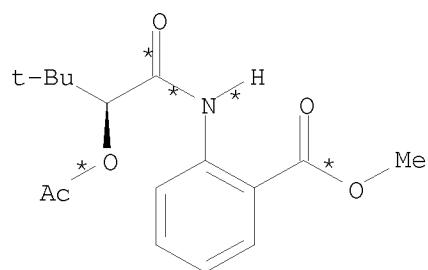
SOL 75-09-2 CH2Cl2

NTE STEREOSELECTIVE

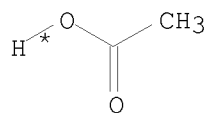
10/ 562,112

RX(70) OF 127 COMPOSED OF RX(3), RX(4), RX(22)

RX(70) 3 G + 3 N + 2 AV ==> AK + AU + AW

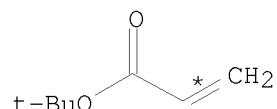


3 G



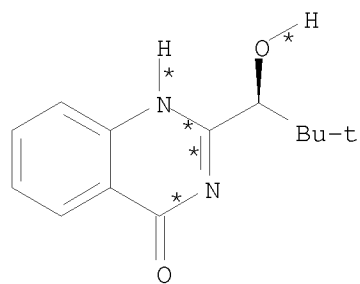
● 1/4 Pb(IV)

3 N

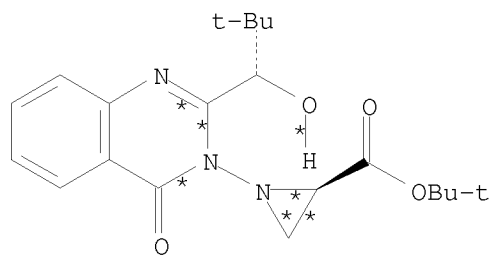


2 AV

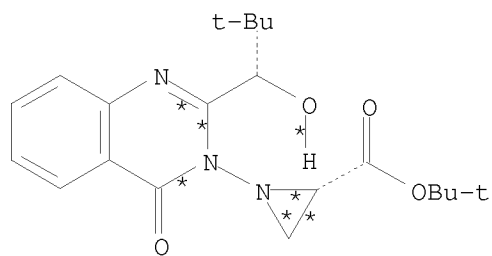
3  
STEPS  
=>



AK  
YIELD 23%



AU  
YIELD 57%(48)



AW  
YIELD 57%(52)

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

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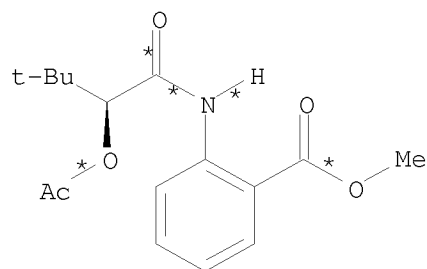
PRO K 182160-10-7  
NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8  
PRO O 182160-08-3  
SOL 865-49-6 CDC13  
NTE STEREOSELECTIVE

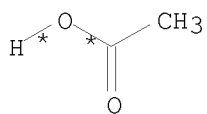
RX(22) RCT O 182160-08-3, AV 1663-39-4  
PRO AK 215546-99-9, AU 215547-03-8, AW 215547-02-7  
SOL 75-09-2 CH2Cl2  
NTE STEREOSELECTIVE

RX(71) OF 127 COMPOSED OF RX(3), RX(4), RX(23)

RX(71) 2 G + 2 N + AV + W ==> AU + AF

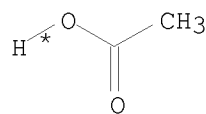


2 G



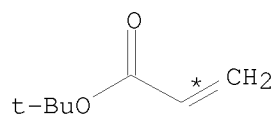
● 1/4 Pb(IV)

N

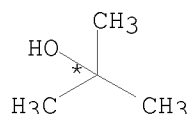


● 1/4 Pb(IV)

N



AV



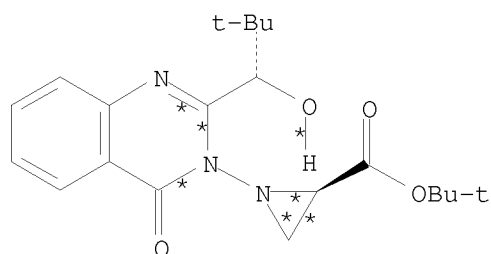
● 1/4 Ti(IV)

W

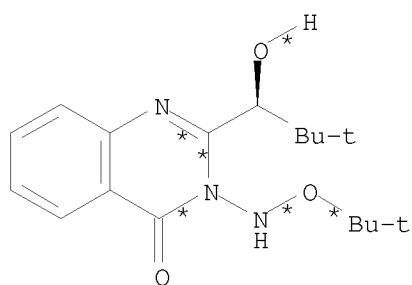
3  
STEPS  
→



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AU  
YIELD 53%



AF  
YIELD 26%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDC13

NTE STEREOSELECTIVE

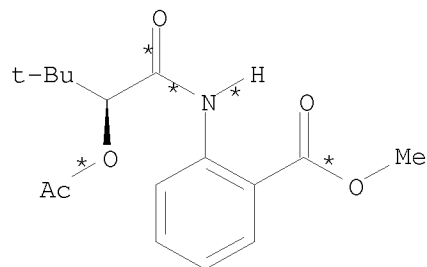
RX(23) RCT O 182160-08-3, AV 1663-39-4, W 3087-39-6

PRO AU 215547-03-8, AF 215546-95-5

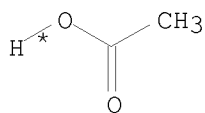
NTE STEREOSELECTIVE

RX(72) OF 127 COMPOSED OF RX(3), RX(4), RX(24)

RX(72) 2 G + 2 N + 2 AX ==> AY + AZ

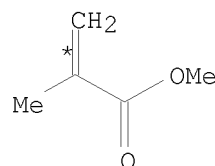


2 G



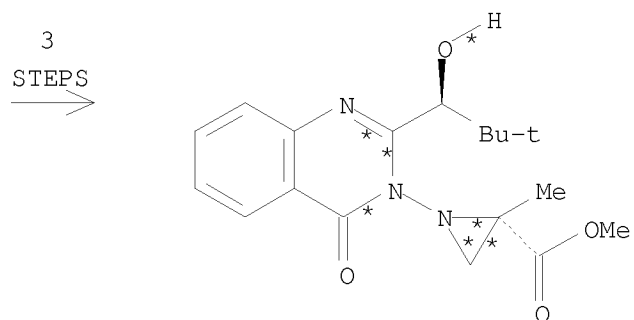
● 1/4 Pb(IV)

2 N

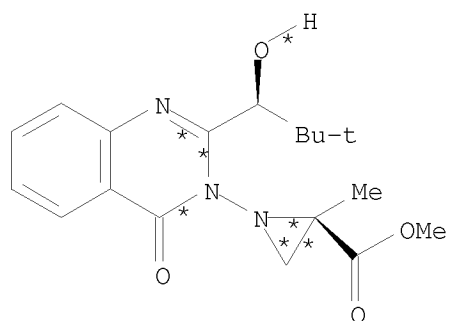


2 AX

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AY  
YIELD 79%(32)



AZ  
YIELD 79%(68)

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4  
SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7  
NTE STEREOSELECTIVE

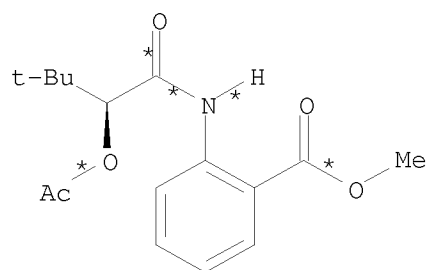
RX(4) RCT K 182160-10-7, N 546-67-8  
PRO O 182160-08-3  
SOL 865-49-6 CDC13  
NTE STEREOSELECTIVE

RX(24) RCT O 182160-08-3, AX 80-62-6  
PRO AY 215547-05-0, AZ 215547-04-9  
SOL 75-09-2 CH2Cl2  
NTE STEREOSELECTIVE

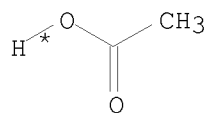
RX(73) OF 127 COMPOSED OF RX(3), RX(4), RX(25)

10/ 562,112

RX(73)      3 G + 3 N + 2 AX + W ==> AY + AZ +  
AF

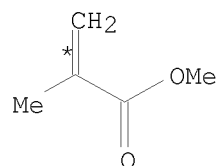


3 G

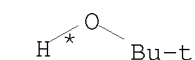


● 1/4 Pb(IV)

3 N



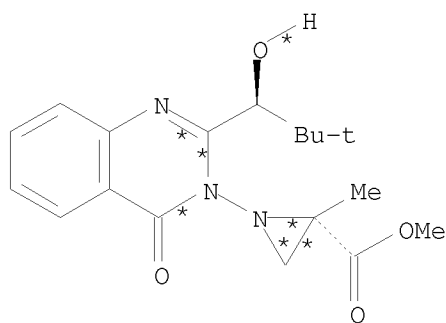
2 AX



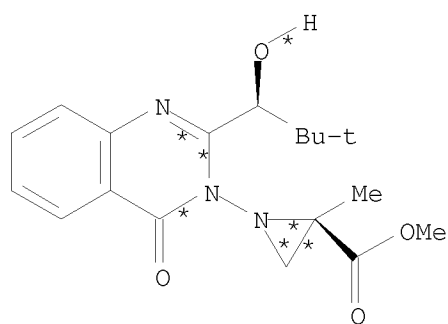
● 1/4 Ti(IV)

W

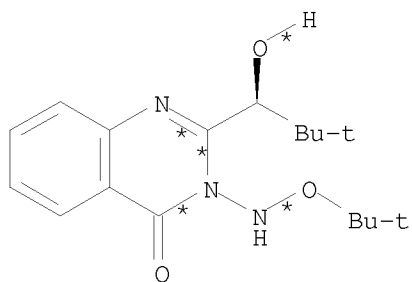
3  
STEPS  
→



AY  
YIELD 45%(87)



AZ  
YIELD 45%(13)



AF  
YIELD 28%

RX(3)      RCT   G 215546-92-2

STAGE(1)

RGT   L 302-01-2 N2H4

SOL   64-17-5 EtOH

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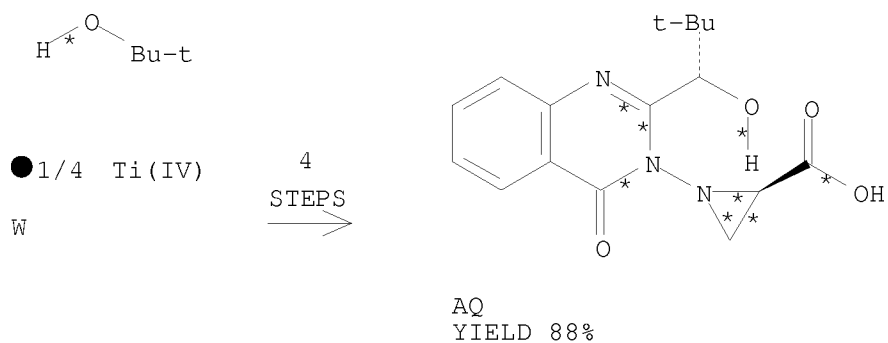
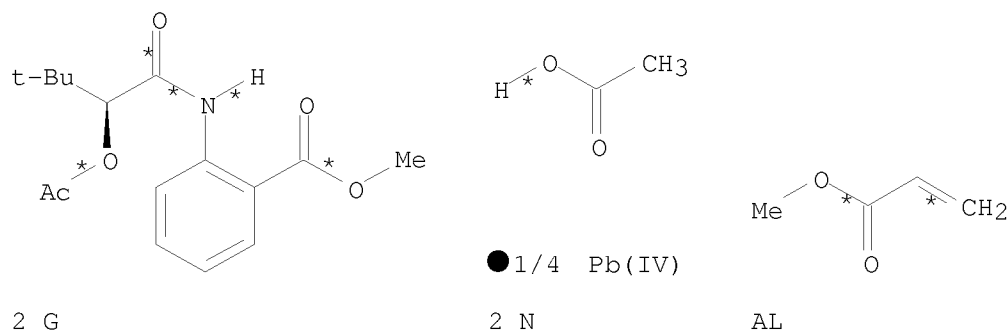
STAGE(2)  
SOL 7732-18-5 Water

PRO K 182160-10-7  
NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8  
PRO O 182160-08-3  
SOL 865-49-6 CDCl3  
NTE STEREOSELECTIVE

RX(25) RCT O 182160-08-3, AX 80-62-6, W 3087-39-6  
PRO AY 215547-05-0, AZ 215547-04-9, AF 215546-95-5  
SOL 75-09-2 CH2Cl2  
NTE STEREOSELECTIVE

RX(96) OF 127 COMPOSED OF RX(3), RX(4), RX(15), RX(19)  
RX(96) 2 G + 2 N + AL + W ==> AQ



RX(3) RCT G 215546-92-2

STAGE(1)  
RGT L 302-01-2 N2H4  
SOL 64-17-5 EtOH

STAGE(2)  
SOL 7732-18-5 Water

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PRO K 182160-10-7  
NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8  
PRO O 182160-08-3  
SOL 865-49-6 CDCl<sub>3</sub>  
NTE STEREOSELECTIVE

RX(15) RCT O 182160-08-3, AL 96-33-3, W 3087-39-6  
PRO AM 215547-00-5, AF 215546-95-5  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
NTE STEREOSELECTIVE

RX(19) RCT AM 215547-00-5

STAGE(1)

RGT AR 1310-73-2 NaOH  
SOL 64-17-5 EtOH, 7732-18-5 Water

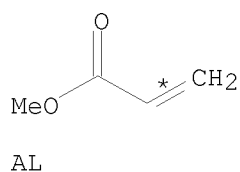
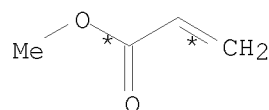
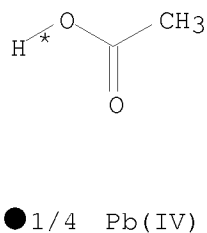
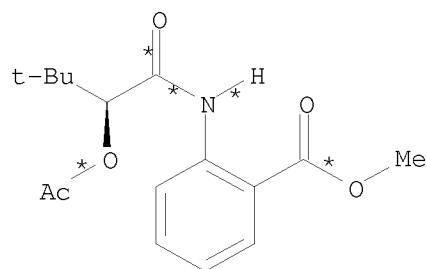
STAGE(2)

RGT AS 7664-93-9 H<sub>2</sub>SO<sub>4</sub>

PRO AQ 215547-06-1  
NTE STEREOSELECTIVE

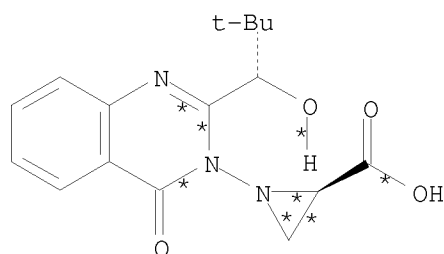
RX(97) OF 127 COMPOSED OF RX(3), RX(4), RX(18), RX(19)

RX(97) 2 G + 2 N + 2 AL ==> AQ



4  
STEPS  
→

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AQ  
YIELD 88%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDCl3

NTE STEREOSELECTIVE

RX(18) RCT O 182160-08-3, AL 96-33-3

PRO AM 215547-00-5, AP 215547-01-6

SOL 75-09-2 CH2Cl2

NTE STEREOSELECTIVE

RX(19) RCT AM 215547-00-5

STAGE(1)

RGT AR 1310-73-2 NaOH

SOL 64-17-5 EtOH, 7732-18-5 Water

STAGE(2)

RGT AS 7664-93-9 H2SO4

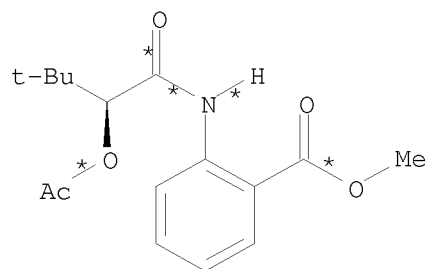
PRO AQ 215547-06-1

NTE STEREOSELECTIVE

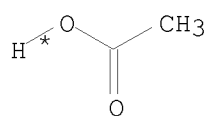
RX(98) OF 127 COMPOSED OF RX(3), RX(4), RX(18), RX(20)

RX(98) 2 G + 2 N + 2 AL ==> AT

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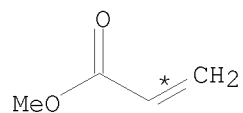


2 G

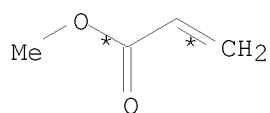


● 1/4 Pb(IV)

2 N

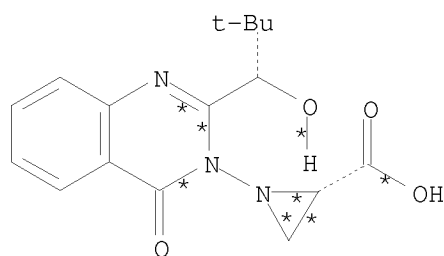


AL



AL

4  
STEPS  
→



AT  
YIELD 88%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDCl3

NTE STEREOSELECTIVE

RX(18) RCT O 182160-08-3, AL 96-33-3

PRO AM 215547-00-5, AP 215547-01-6

SOL 75-09-2 CH2Cl2

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NTE STEREOSELECTIVE

RX(20) RCT AP 215547-01-6

STAGE(1)

RGT AR 1310-73-2 NaOH

SOL 64-17-5 EtOH, 7732-18-5 Water

STAGE(2)

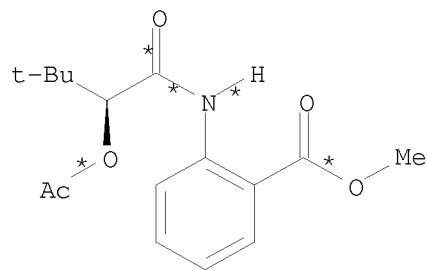
RGT AS 7664-93-9 H2SO4

PRO AT 215547-07-2

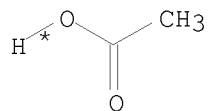
NTE STEREOSELECTIVE

RX(99) OF 127 COMPOSED OF RX(3), RX(4), RX(22), RX(21)

RX(99) 3 G + 3 N + 2 AV ==> AQ

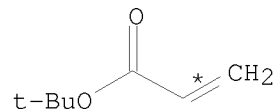


3 G

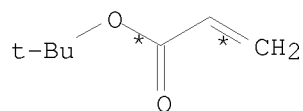


1/4 Pb(IV)

3 N

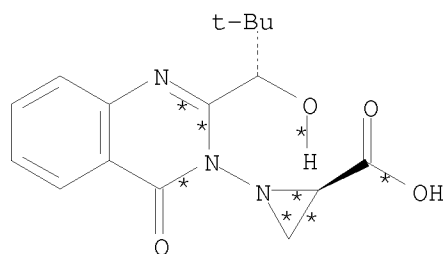


AV



AV

4  
STEPS  
→



AQ

YIELD 56%

RX(3) RCT G 215546-92-2



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STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDCl3

NTE STEREOSELECTIVE

RX(22) RCT O 182160-08-3, AV 1663-39-4

PRO AK 215546-99-9, AU 215547-03-8, AW 215547-02-7

SOL 75-09-2 CH2Cl2

NTE STEREOSELECTIVE

RX(21) RCT AU 215547-03-8

STAGE(1)

RGT AR 1310-73-2 NaOH

SOL 64-17-5 EtOH, 7732-18-5 Water

STAGE(2)

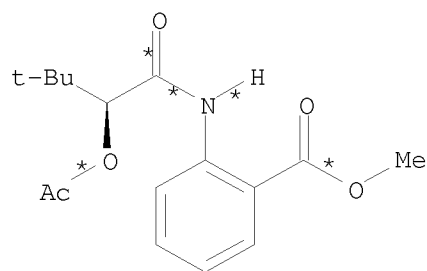
RGT AS 7664-93-9 H2SO4

PRO AQ 215547-06-1

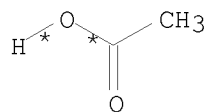
NTE STEREOSELECTIVE

RX(100) OF 127 COMPOSED OF RX(3), RX(4), RX(23), RX(21)

RX(100) 2 G + 2 N + AV + W ==> AQ

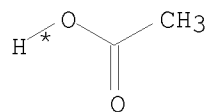


2 G



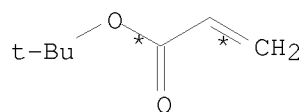
● 1/4 Pb(IV)

N



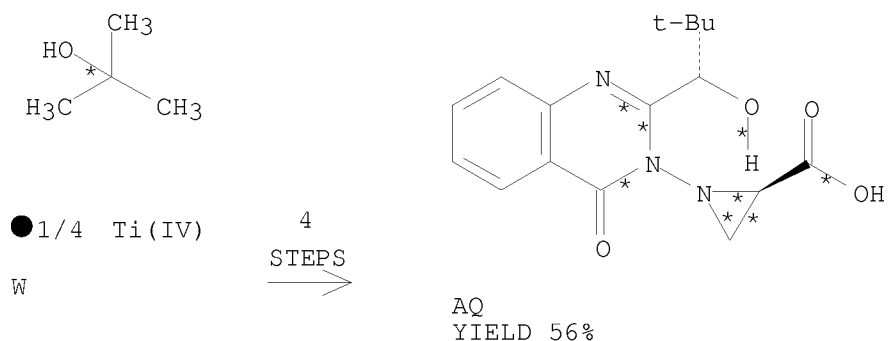
● 1/4 Pb(IV)

N



AV

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RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDCl3

NTE STEREOSELECTIVE

RX(23) RCT O 182160-08-3, AV 1663-39-4, W 3087-39-6

PRO AU 215547-03-8, AF 215546-95-5

NTE STEREOSELECTIVE

RX(21) RCT AU 215547-03-8

STAGE(1)

RGT AR 1310-73-2 NaOH

SOL 64-17-5 EtOH, 7732-18-5 Water

STAGE(2)

RGT AS 7664-93-9 H2SO4

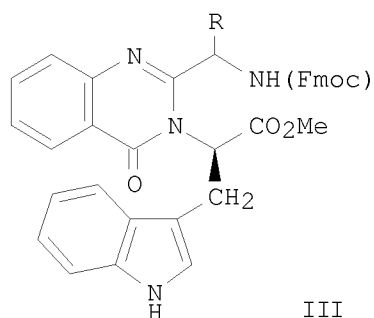
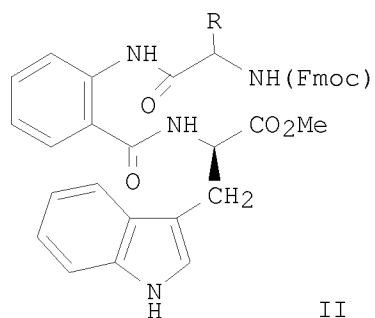
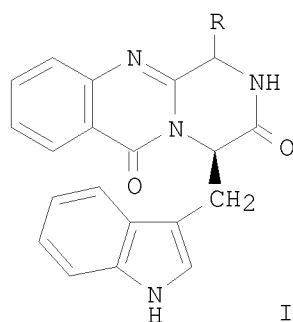
PRO AQ 215547-06-1

NTE STEREOSELECTIVE

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 123 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 128:257597 CASREACT  
TITLE: Total Synthesis of the Quinazoline Alkaloids  
(-)-Fumiquinazoline G and (-)-Fiscalin B  
AUTHOR(S): Wang, Haishan; Ganesan, A.

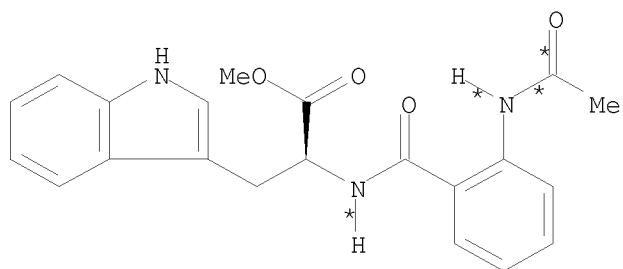
CORPORATE SOURCE: Institute of Molecular and Cell Biology, National  
 University of Singapore, Singapore, 117609, Singapore  
 SOURCE: Journal of Organic Chemistry (1998), 63(8), 2432-2433  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB (-)-Fumiquinazoline G (I; R =  $\beta$ -Me) and (-)-fiscalin B (I; R =  $\alpha$ -CHMe<sub>2</sub>) were synthesized in four and five steps resp. from D-tryptophan Me ester. The key transformation involved dehydrative cyclization of linear tripeptides II (Fmoc = 9-fluorenylmethoxycarbonyl, R =  $\beta$ -Me,  $\alpha$ -CHMe<sub>2</sub>, resp.) to quinazolin-4-ones III. The methodol. is also applicable to the synthesis of quinazolinones with sterically bulky 2,3-substitution.

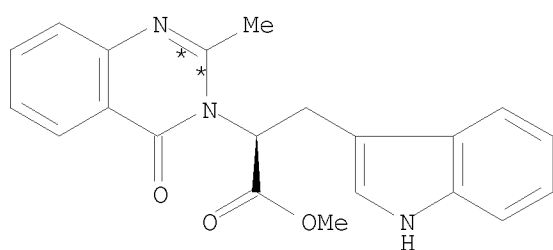
RX(3) OF 20 I ==> J

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I

(3)  $\Rightarrow$

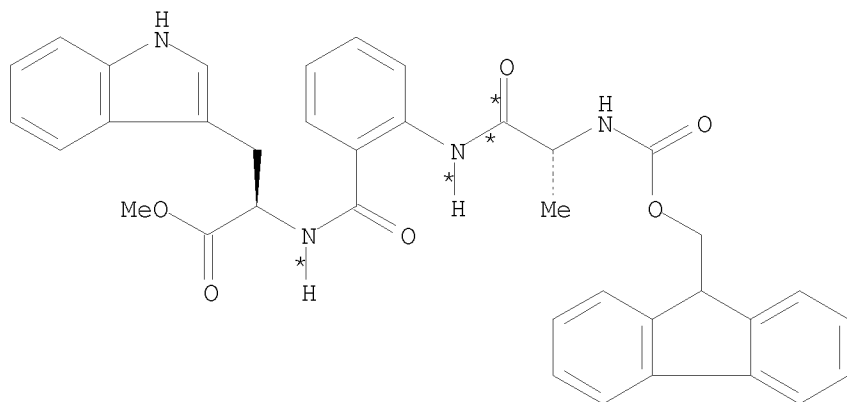


J

YIELD 99%

RX(3) RCT I 205042-92-8  
 RGT K 603-35-0 PPh3, L 7553-56-2 I2, M 7087-68-5 EtN(Pr-i)2  
 PRO J 205042-90-6  
 SOL 75-09-2 CH2Cl2

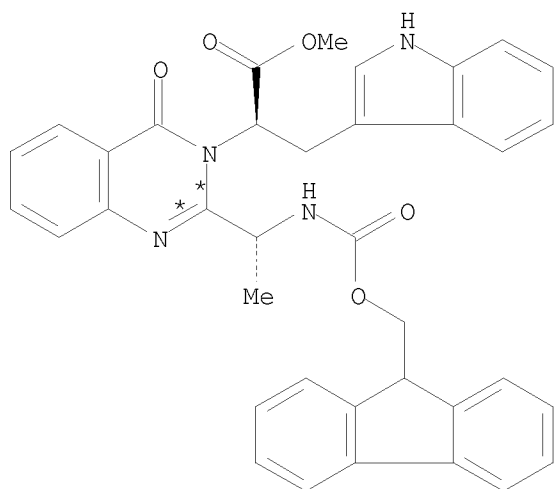
RX(6) OF 20 ...S ==> A...



S

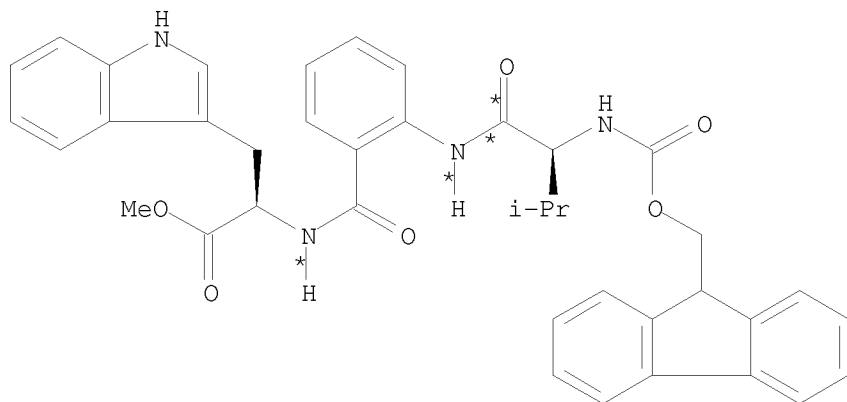
(6)  $\Rightarrow$

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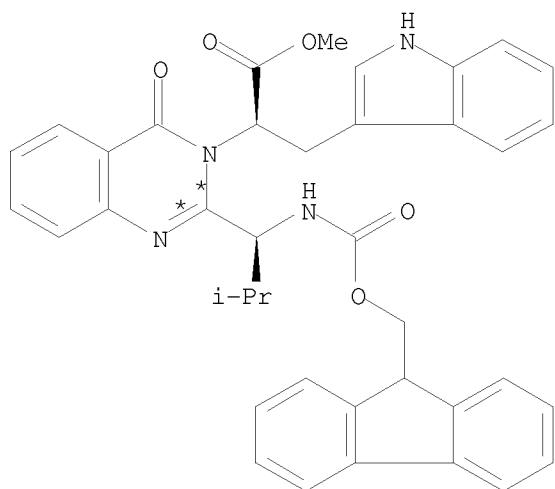


RX(6) RCT S 205042-95-1  
RGT K 603-35-0 PPh3, L 7553-56-2 I2, M 7087-68-5 EtN(Pr-i)2  
PRO A 205042-96-2  
SOL 75-09-2 CH2Cl2  
NTE key step

RX(8) OF 20 ...W ==> X



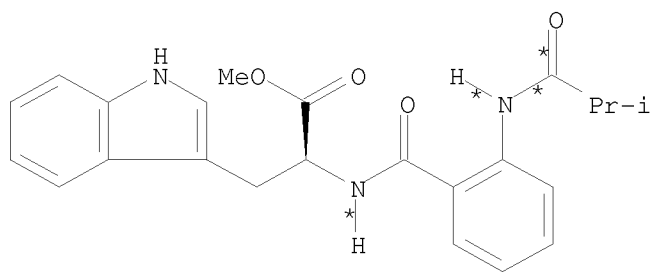
10/ 562,112



X  
YIELD 82%

RX(8) RCT W 205042-97-3  
RGT K 603-35-0 PPh3, L 7553-56-2 I2, M 7087-68-5 EtN(Pr-i)2  
PRO X 205042-98-4  
SOL 75-09-2 CH2Cl2  
NTE key step

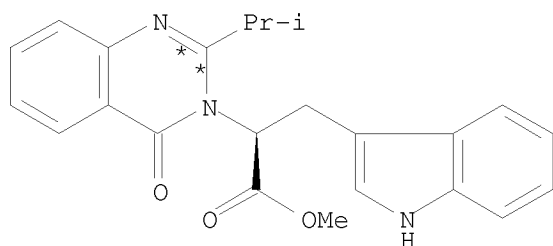
RX(10) OF 20 AA ==> AB



AA

(10)  
→

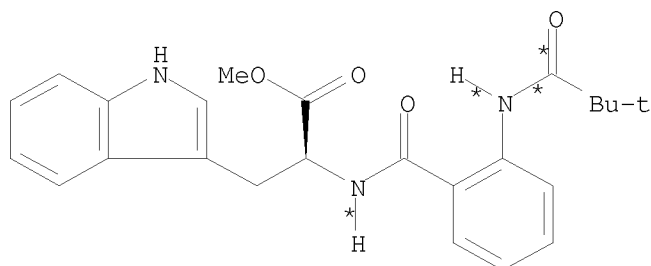
10/ 562,112



AB  
YIELD 88%

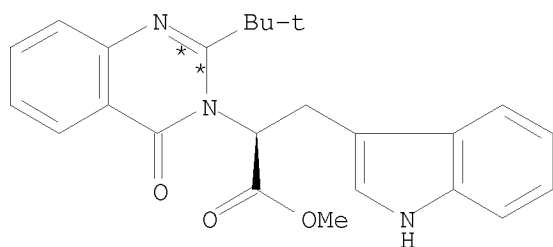
RX(10) RCT AA 205043-03-4  
RGT K 603-35-0 PPh3, L 7553-56-2 I2, M 7087-68-5 EtN(Pr-i)2  
PRO AB 205043-02-3  
SOL 75-09-2 CH2Cl2

RX(11) OF 20 AC ==> AD



AC

(11)  
→



AD  
YIELD 17%

RX(11) RCT AC 205043-06-7  
RGT K 603-35-0 PPh3, L 7553-56-2 I2, M 7087-68-5 EtN(Pr-i)2  
PRO AD 205043-04-5  
SOL 75-09-2 CH2Cl2

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 124 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 128:127982 CASREACT

TITLE: An improved synthesis of 2,3-disubstituted 4(3H)-quinazolinones from 2-acylamino-N-arylbenzamides

AUTHOR(S): Acharya, Debi Prasad; Chattopadhyay, Subhagata

CORPORATE SOURCE: Department of Chemistry, Jadavpur University, Calcutta, 700 032, India

SOURCE: Indian Journal of Heterocyclic Chemistry (1997), 7(2), 101-104

CODEN: IJCHEI; ISSN: 0971-1627

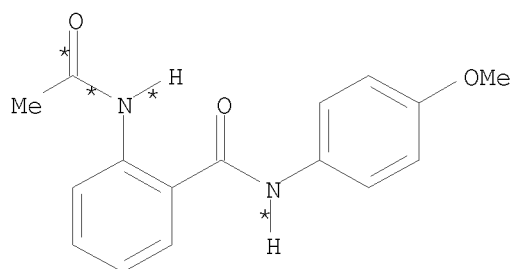
PUBLISHER: Lucknow University, Dep. of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

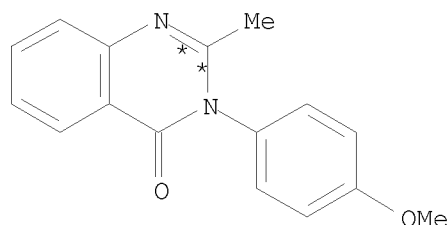
AB 2-Acylamino-N-arylbenzamides on refluxing with TsOH in benzene or MeCN solution undergo smooth cyclodehydration to 2,3-disubstituted 4(3H)-quinazolinones. A convenient procedure for converting isatoic anhydride to 2-amino-N-aryl(alkyl)benzamides is also reported.

RX(10) OF 18 V ==> W



V

(10)



W

YIELD 88%

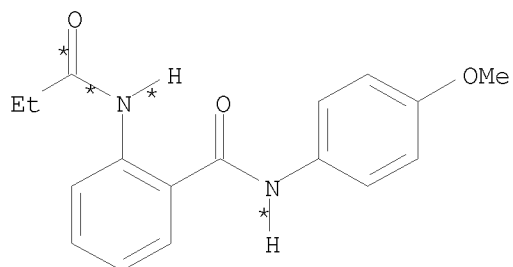
RX(10) RCT V 59525-22-3  
RGT X 104-15-4 TsOH  
PRO W 30507-16-5



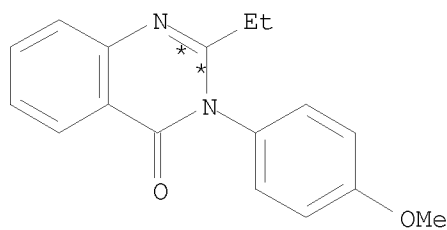
10/ 562,112

SOL 71-43-2 Benzene

RX(11) OF 18 Z ==> AA



Z

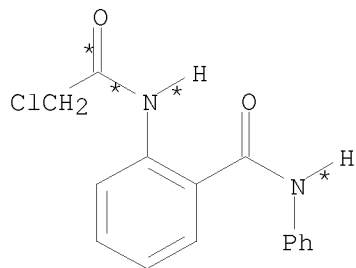


AA

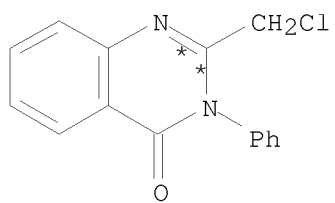
YIELD 71%

RX(11) RCT Z 25628-95-9  
RGT X 104-15-4 TsOH  
PRO AA 50498-62-9  
SOL 71-43-2 Benzene

RX(12) OF 18 AB ==> AC



AB



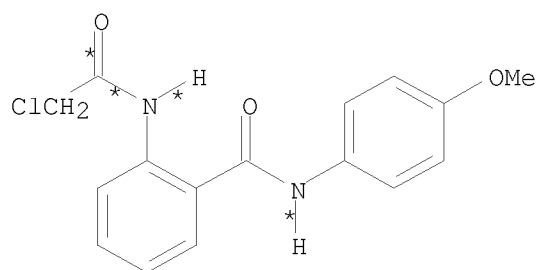
AC

YIELD 68%

10/ 562,112

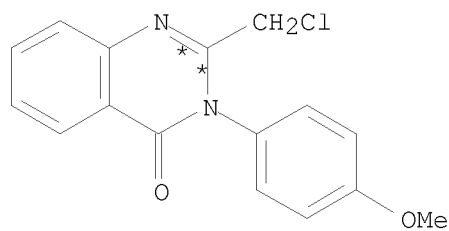
RX(12)      RCT    AB 18871-29-9  
              RGT    X 104-15-4 TsOH  
              PRO    AC 22312-77-2  
              SOL    71-43-2 Benzene

RX(13) OF 18      AD    ==>    AE



AD

(13)  
→

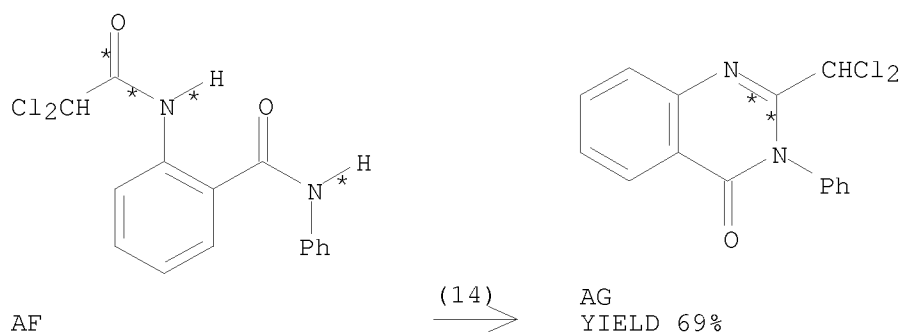


AE  
YIELD 79%

RX(13)      RCT    AD 22312-68-1  
              RGT    X 104-15-4 TsOH  
              PRO    AE 22312-82-9  
              SOL    71-43-2 Benzene

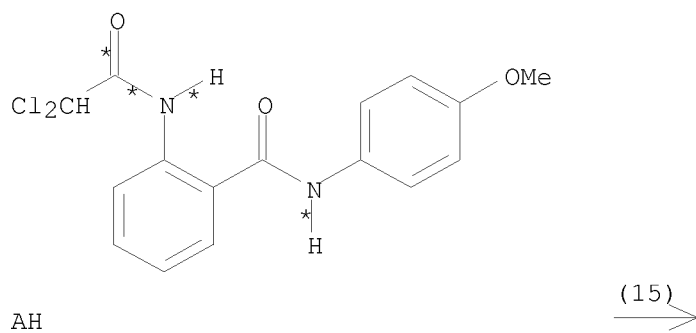
RX(14) OF 18      AF    ==>    AG

10/ 562,112



RX(14)      RCT    AF 202137-04-0  
              RGT    X 104-15-4 TsOH  
              PRO    AG 202137-02-8  
              SOL    71-43-2 Benzene

RX(15) OF 18      AH ==> AI

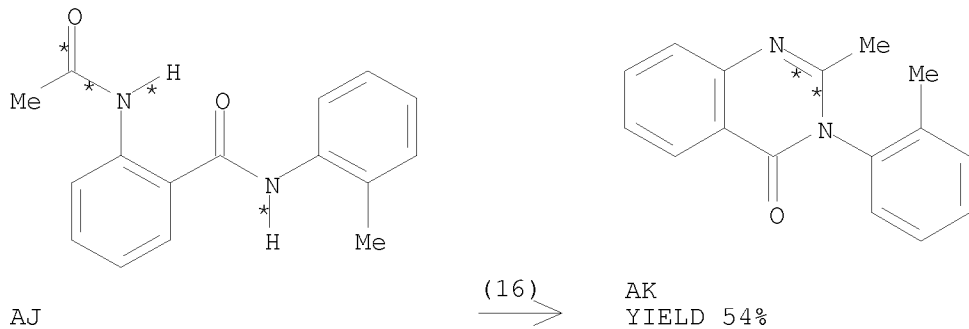


AI  
YIELD 74%

RX(15)      RCT    AH 202137-05-1  
              RGT    X 104-15-4 TsOH  
              PRO    AI 33227-62-2  
              SOL    71-43-2 Benzene

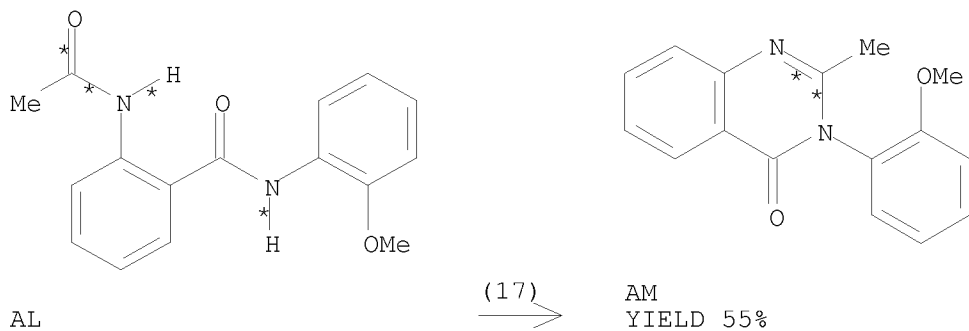
10/ 562,112

RX(16) OF 18      AJ    ==>    AK



RX(16)	RCT	AJ 70180-39-1
	RGT	X 104-15-4 TsOH
	PRO	AK 72-44-6
	SOL	71-43-2 Benzene

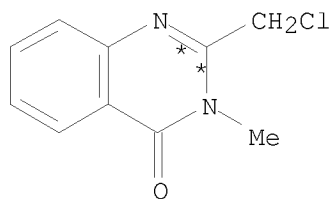
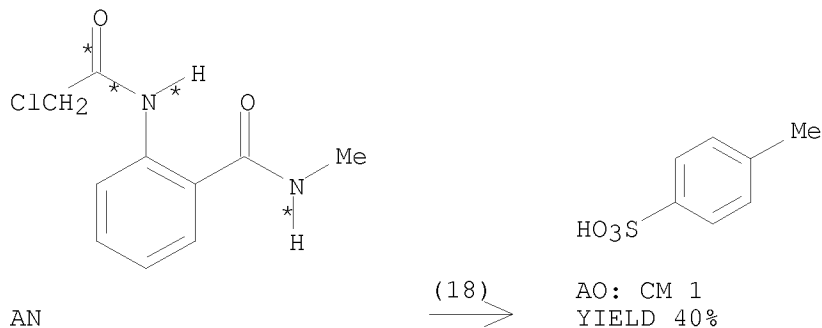
RX(17) OF 18 AL ==&gt; AM



RX(17)	RCT	AL 92966-82-0
	RGT	X 104-15-4 TsOH
	PRO	AM 4260-28-0
	SOL	71-43-2 Benzene

RX(18) OF 18      AN      ==>      AO

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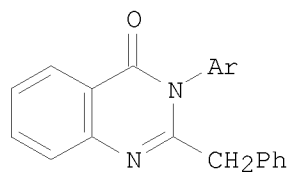
AO: CM 2  
YIELD 40%

RX (18)	RCT	AN 53824-91-2
	RGT	X 104-15-4 TsOH
	PRO	AO 202137-03-9
	SOL	71-43-2 Benzene

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L3      ANSWER 125 OF 258      CASREACT  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:              128:102054  CASREACT
TITLE:                          Synthesis of some new quinazolin-4(3H)-ones as
                                possible antimicrobial agents
AUTHOR(S):                      Mishra, Pradeep; Jain, Sanmati K.; Jain, Sandeep
CORPORATE SOURCE:               Dep. Pharmaceutical Sci., Dr. Harisingh Gour
                                Vishwavidyalaya, Sagar, 470 003, India
SOURCE:                          Journal of the Indian Chemical Society (1997), 74(10),
                                816-817
                                CODEN: JICSAH; ISSN: 0019-4522
PUBLISHER:                      Indian Chemical Society
DOCUMENT TYPE:                  Journal
LANGUAGE:                       English
GI
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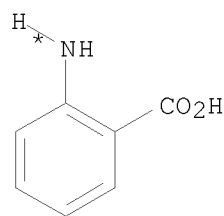
10/ 562,112



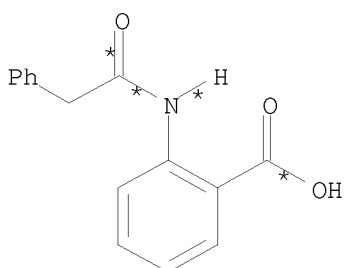
I

AB Reaction of anthranilic acid with phenacetyl chloride gave o-(phenacetyl-amino)benzoic acid which on cyclization in presence of acetic anhydride gave 2-phenylmethyl-3,1-benzoxazin-4-one. Condensation of the latter with aromatic amines gave title compds. I (Ar = 3-C<sub>6</sub>H<sub>4</sub>OH, Ph, 2-C<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H, 4-C<sub>6</sub>H<sub>4</sub>Br, 2-C<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>, 4-C<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H, 3-C<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>, 4-C<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>). Bactericidal activity of some of the compds. prepared is discussed.

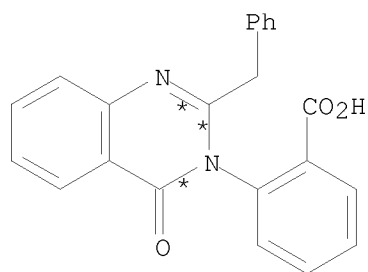
RX(2) OF 3 ...A + C ==> D



A



C



D

YIELD 48%

RX(2) RCT A 118-92-3, C 28565-98-2  
 RGT E 64-19-7 AcOH, F 108-24-7 Ac2O  
 PRO D 201293-02-9  
 NTE 4-6 H

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

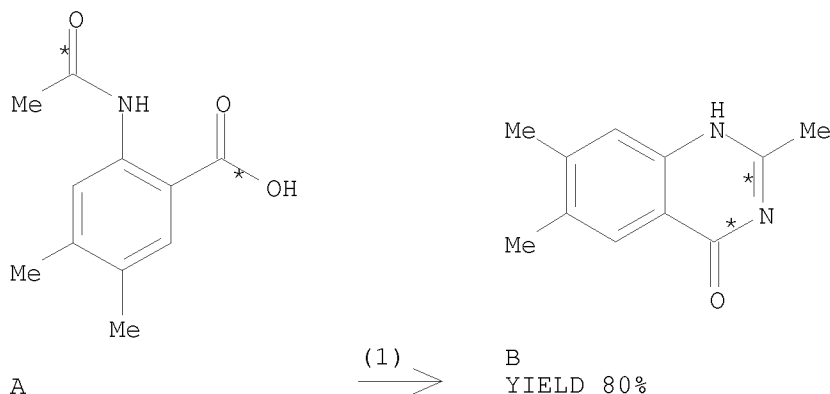
L3 ANSWER 126 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 127:205586 CASREACT  
 TITLE: Preparation of 5,6-dihydro-3H-pyrimidin-4-one derivatives.  
 INVENTOR(S): Bhattacharya, Apurba; Allen, Diane E.  
 PATENT ASSIGNEE(S): Hoechst Celanese Corp., USA  
 SOURCE: PCT Int. Appl., 29 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9728132	A1	19970807	WO 1997-US1860	19970130
W: CN, JP				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5763608	A	19980609	US 1996-595885	19960205
IN 182629	A1	19990522	IN 1997-CA107	19970120
PRIORITY APPLN. INFO.:			US 1996-595885	19960205

OTHER SOURCE(S): MARPAT 127:205586

AB 5,6-Dihydro-3H-pyrimidin-4-one derivs. were prepared by (a) dehydrating N-acyl  $\beta$ -amino acid derivs. in the presence of a dehydrating agent and an organic solvent to form oxazones; (b) adding a carboxylic acid and a primary amine salt of a carboxylic acid to said oxazones to form a mixture; (c) distilling azeotropically said mixture to remove the dehydrating agent and organic solvent; and (d) heating the product of step (c). Thus, 2-acetyl-amino-4,5-dimethylbenzoic acid (preparation given) was refluxed 3 h with Ac<sub>2</sub>O and heptane; NH<sub>4</sub>OAc was added followed by distillation of heptane, addition of AcOH, continued distillation, and reflux for 12 h to give 80% 2,6,7-trimethyl-4(3H)-quinazolinone.

RX(1) OF 1 A ==> B



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RX(1) RCT A 15089-80-2

STAGE(1)

RGT C 108-24-7 Ac2O  
SOL 142-82-5 Heptane

STAGE(2)

RGT D 631-61-8 NH4OAc, E 64-19-7 AcOH

PRO B 119063-78-4

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 127 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 127:190527 CASREACT  
TITLE: Three-step process for preparing anthranilic acids  
from anilines  
INVENTOR(S): Bhattacharya, Apurba; Allen, Diane E.  
PATENT ASSIGNEE(S): Hoechst Celanese Corp., USA  
SOURCE: PCT Int. Appl., 29 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

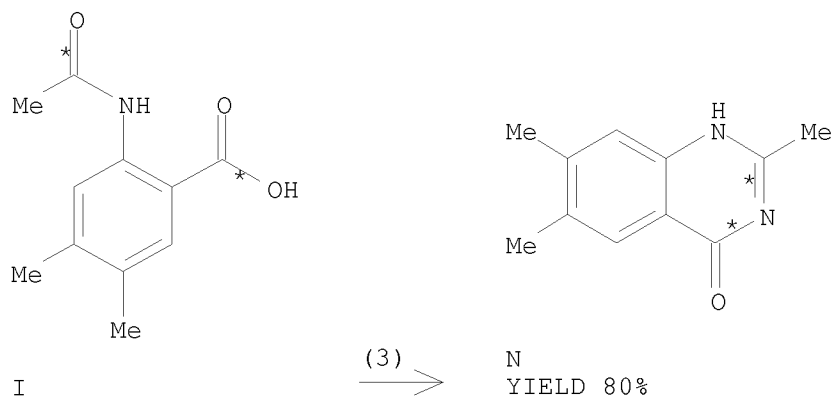
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9728118	A1	19970807	WO 1997-US1862	19970130
W: CN, JP				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRIORITY APPLN. INFO.:		US 1996-596536 19960205		
OTHER SOURCE(S):		MARPAT 127:190527		

AB Anthranilic acids, useful as cyclocondensation intermediates in the preparation of 4-quinazolinones, are prepared in high yield and selectivity by: (a) acylating an aniline with an acylation agent (e.g., Ac2O) to form the corresponding amide; (b) subjecting the acetylated intermediate to halogenation in the presence of an oxidizing agent (e.g., H2O2) to form an ortho-halogenated aniline amide; and (c) subjecting the ortho-halogenated aniline amide to carbonylation to form the anthranilic acid. Thus, 3,4-dimethylaniline was acylated with Ac2O, brominated with Br2 and H2O2, and carbonylated in the presence of CO, PPh3, and (PPh3)2PdCl2, producing 2-(acetylamino)-4,5-dimethylbenzoic acid.

RX(3) OF 6 ...I ==> N



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RX(3) RCT I 15089-80-2

STAGE(1)

SOL 142-82-5 Heptane, 108-24-7 Ac2O

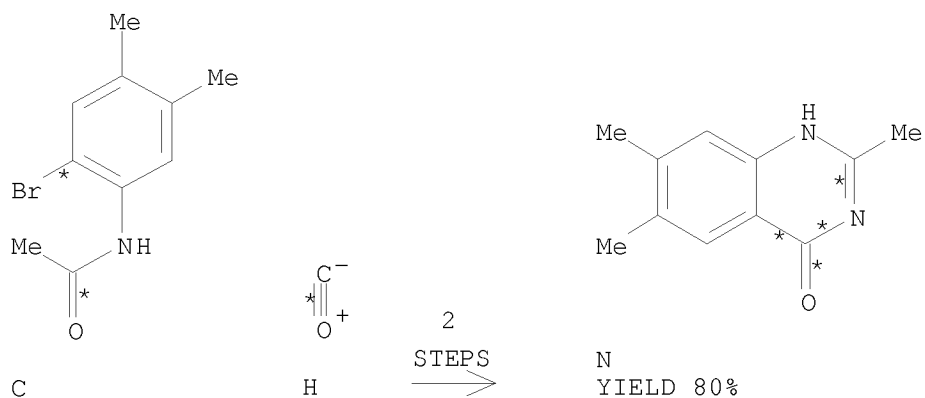
STAGE(2)

RGT O 631-61-8 NH4OAc

PRO N 119063-78-4

RX(5) OF 6 COMPOSED OF RX(2), RX(3)

RX(5) C + H ==> N



RX(2) RCT C 22364-28-9, H 630-08-0

RGT J 102-82-9 Bu3N

PRO I 15089-80-2

CAT 7439-95-4 Mg, 13965-03-2 PdCl2(PPh3)2

SOL 108-88-3 PhMe

RX(3) RCT I 15089-80-2

STAGE(1)

SOL 142-82-5 Heptane, 108-24-7 Ac2O

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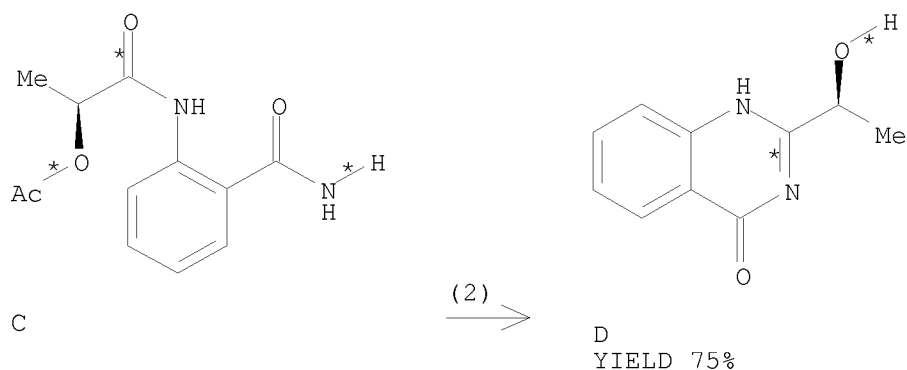
STAGE(2)  
RGT O 631-61-8 NH4OAc

PRO N 119063-78-4

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 128 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 127:162006 CASREACT  
TITLE: Comments on the asymmetric synthesis of chrysogine  
AUTHOR(S): Bergman, Jan  
CORPORATE SOURCE: Department Organic Chemistry, Institute Biosciences  
Novum, Huddinge, S-141 57, Swed.  
SOURCE: Journal of Chemical Research, Synopses (1997), (6),  
224  
CODEN: JRPSDC; ISSN: 0308-2342  
PUBLISHER: Royal Society of Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The absolute configuration of the mold metabolite chrysogine,  
(S)-(-)-2-(1-hydroxyethyl)quinazolin-4(3H)-one, was first determined by asym.  
synthesis in 1990 and not in 1996 as recently claimed.

RX(2) OF 3 ...C ==> D



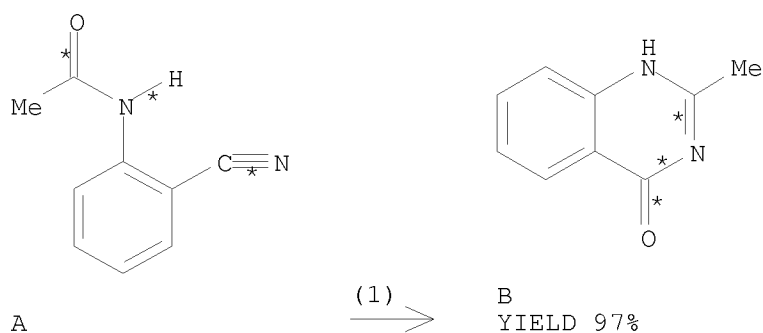
RX(2) RCT C 129768-43-0  
PRO D 42599-89-3

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 129 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 126:330589 CASREACT  
TITLE: Synthesis of quinazolin-4(3H)-ones from  
o-amidobenzonitriles using urea-hydrogen peroxide  
AUTHOR(S): Bandgar, B. P.

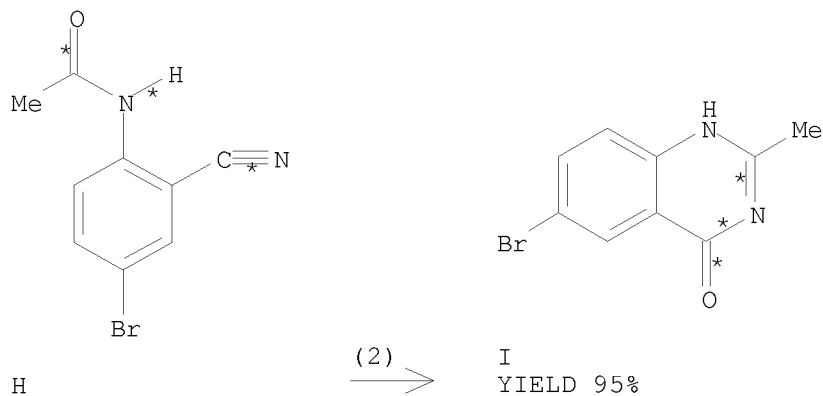
CORPORATE SOURCE: Department of Chemistry, Post Graduate and Research Centre, R. B. N. B. College, Shrirampur, 413709, India  
 SOURCE: Synthetic Communications (1997), 27(12), 2065-2068  
 CODEN: SYNCAV; ISSN: 0039-7911  
 PUBLISHER: Dekker  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Synthesis of quinazolin-4(3H)-ones from o-amidobenzonitriles has been carried out by using urea-hydrogen peroxide as a mild, stable and non-hazardous reagent.

RX(1) OF 7 A ==&gt; B



RX(1) RCT A 25116-00-1  
 RGT C 57-13-6 Urea, D 7722-84-1 H2O2  
 PRO B 1769-24-0  
 CAT 584-08-7 K2CO3  
 SOL 7732-18-5 Water, 67-64-1 Me2CO

RX(2) OF 7 H ==&gt; I

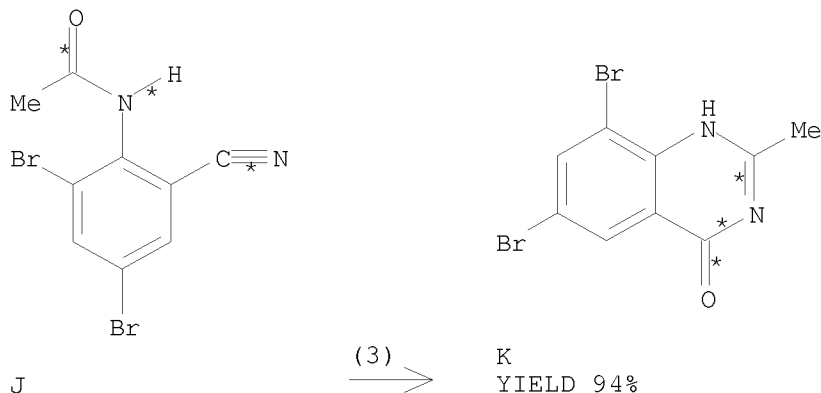


RX(2) RCT H 189634-99-9  
 RGT C 57-13-6 Urea, D 7722-84-1 H2O2  
 PRO I 5426-59-5  
 CAT 584-08-7 K2CO3

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SOL 7732-18-5 Water, 67-64-1 Me2CO

RX(3) OF 7 J ==> K



RX(3) RCT J 189635-00-5  
RGT C 57-13-6 Urea, D 7722-84-1 H2O2  
PRO K 82326-77-0  
CAT 584-08-7 K2CO3  
SOL 7732-18-5 Water, 67-64-1 Me2CO

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

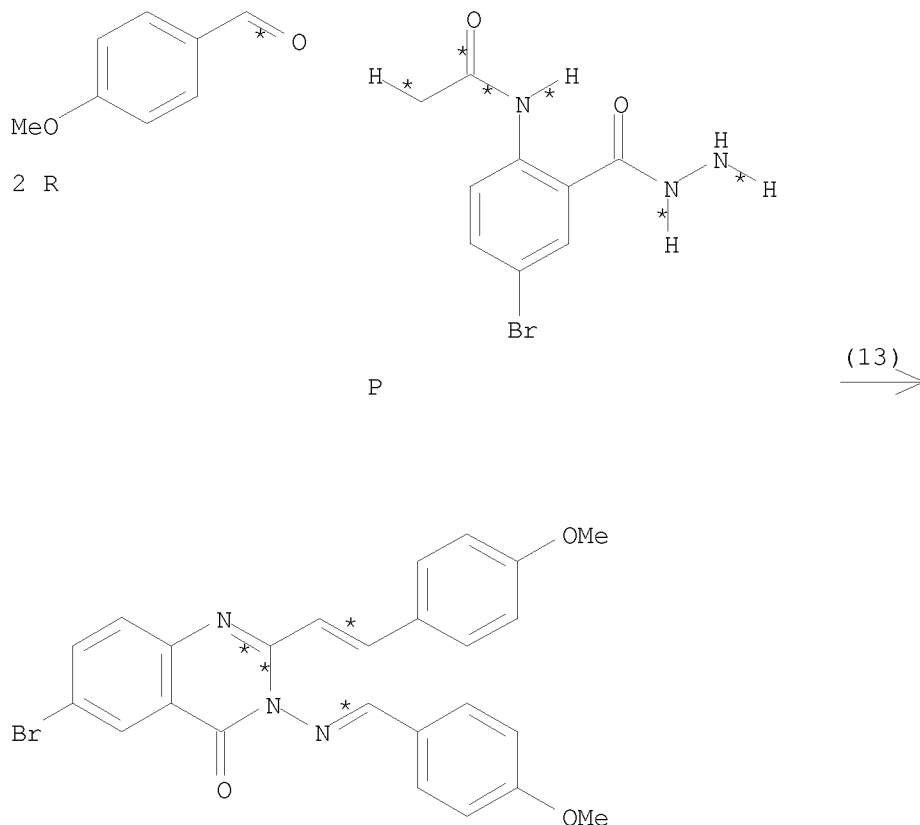
L3 ANSWER 130 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 125:10738 CASREACT  
TITLE: Chemoselectivity of  
6-bromo-2-methyl-3,1-benzoxazin-4-one towards amines,  
Schiff bases, and azines  
AUTHOR(S): Derbala, H. A.  
CORPORATE SOURCE: CHem. Dep., Ain Shams Univ., Cairo, Egypt  
SOURCE: Monatshefte fuer Chemie (1996), 127(1), 103-10  
CODEN: MOCMB7; ISSN: 0026-9247  
PUBLISHER: Springer  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB 6-Bromo-2-methyl-3,1-benzoxazin-4-one (1) undergoes an unusual cleavage at position 4 when it is allowed to react with o-phenylenediamine or anthranilic acid in dry benzene to give the corresponding compds. I, II, III, IV, resp. The reaction of 1 with Schiff bases and azines results in the formation of the compds. V [R, R' given: H, H; p-MeO, H; H, p-Cl; 3, 4-(MeO)2, H] and VI (R2-H, p-MeO), resp. The reaction involves a cleavage of the Schiff base or the azine into its amine and

arylidene moieties which are smoothly incorporated into 1 via nucleophilic attack of the amine at position 4 and condensation of the aldehyde with a reactive Me group, at position 2 resp. No displacement of the arylidene segment was observed

RX(13) OF 14 ...2 R + P ==> S



S  
YIELD 63%

RX(13) RCT R 123-11-5, P 71822-95-2  
RGT K 64-19-7 AcOH, L 127-09-3 AcONa  
PRO S 175877-95-9  
NTE 6 H

L3 ANSWER 131 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 122:81279 CASREACT  
TITLE: Facile synthesis of  
2-alkyl-3-aryl-4(3H)-quinazolinones  
AUTHOR(S): Ramana, D. V.; Kantharaj, E.  
CORPORATE SOURCE: Department Chemistry, Indian Institute Technology,  
Madras, 600 036, India  
SOURCE: Indian Journal of Heterocyclic Chemistry (1994), 3(4),

215-18

CODEN: IJCHEI; ISSN: 0971-1627

DOCUMENT TYPE:

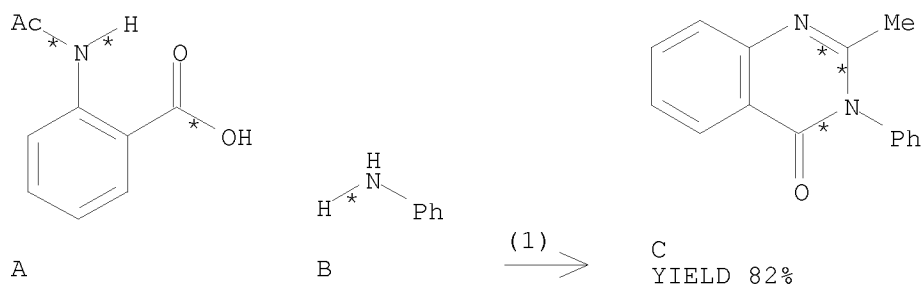
Journal

LANGUAGE:

English

AB The synthesis of 2-alkyl-3-aryl-4(3H)-quinazolinones was achieved in good yields under mild conditions by reaction of N-acylanthranilic acids with tosyl chloride in pyridine at room temperature followed by the addition of amine.

RX(1) OF 4 A + B ==&gt; C



RX(1) RCT A 89-52-1

STAGE(1)

RGT D 98-59-9 TsCl

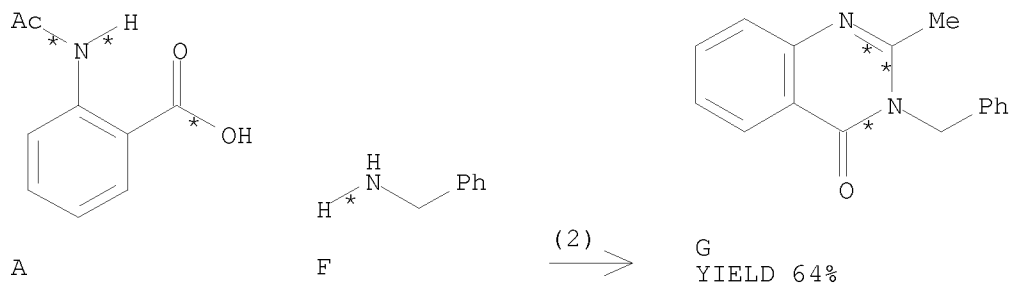
SOL 110-86-1 Pyridine

STAGE(2)

RCT B 62-53-3

PRO C 2385-23-1

RX(2) OF 4 A + F ==&gt; G



RX(2) RCT A 89-52-1

STAGE(1)

RGT D 98-59-9 TsCl

SOL 110-86-1 Pyridine

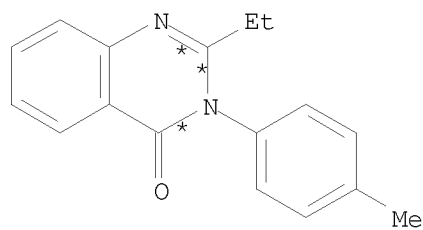
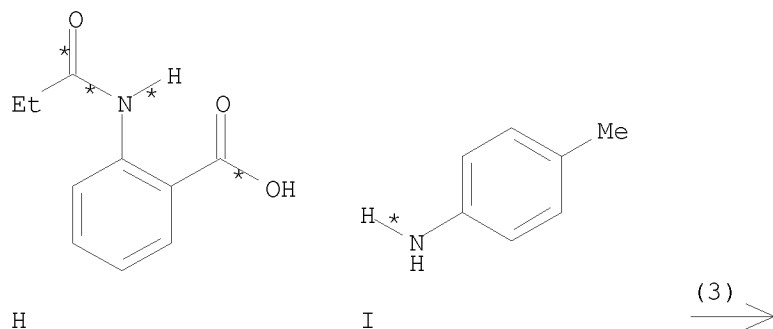
STAGE(2)

RCT F 100-46-9

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PRO G 4260-34-8

RX(3) OF 4 H + I ==> J



J  
YIELD 70%

RX(3) RCT H 19165-26-5

STAGE(1)

RGT D 98-59-9 TsCl

SOL 110-86-1 Pyridine

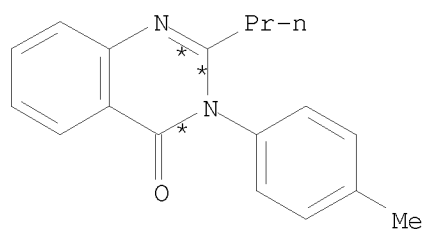
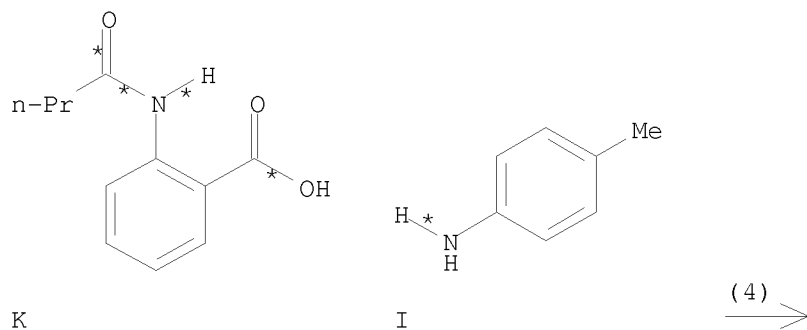
STAGE(2)

RCT I 106-49-0

PRO J 50498-61-8

RX(4) OF 4 K + I ==> L

10/ 562,112



YIELD 78%

RX(4) RCT K 6328-94-5

STAGE(1)

RGT D 98-59-9 TsCl

SOL 110-86-1 Pyridine

STAGE(2)

RCT I 106-49-0

PRO L 84312-85-6

L3 ANSWER 132 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 121:255825 CASREACT

TITLE: Process for the preparation of 2-alkyl-3,5,6,7- or 8-substituted-4-(3H)-quinazolinones via heterocyclization of N-acylanthranilic acids with ethyl chloroformate and ammonia/amine

INVENTOR(S): Mohan, Arthur G.; D, Antuono, Joseph III.

PATENT ASSIGNEE(S): American Cyanamid Company, USA

SOURCE: U.S., 6 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

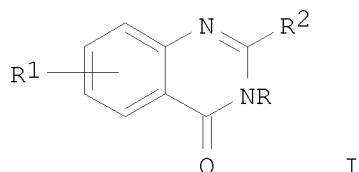
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

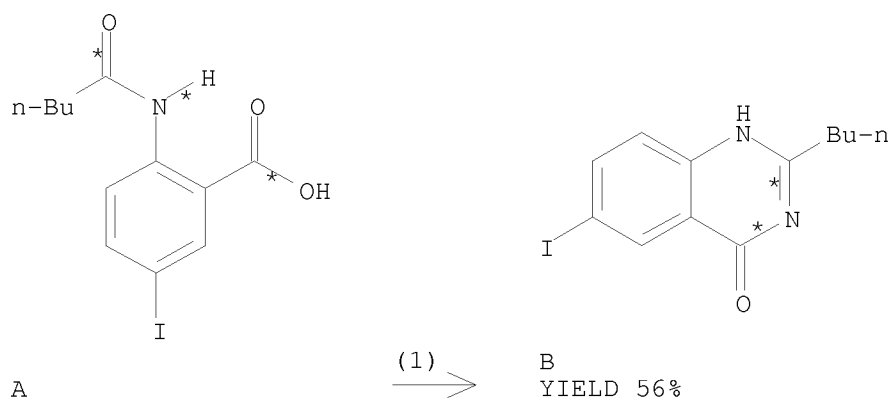


PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 5342944	A	19940830	US 1993-92850	19930719
PRIORITY APPLN. INFO.:			US 1993-92850	19930719
OTHER SOURCE(S):		MARPAT 121:255825		
GI				



AB A novel process for producing 2-alkyl-3,5,6,7 or 8-substituted-4(3H)-quinazolinones of the formula I (R is selected from H, straight or branched alkyl of 1 to 9 carbon atoms, Ph, substituted Ph, etc.; R1 is a straight or branched alkyl of 1 to 9 carbon atoms, optionally substituted with a substituent selected from H, straight chain alkyl of 1 to 4 carbon atoms, Ph, substituted Ph, etc.; R2 is a straight chain alkyl of 1 to 6 carbon atoms) consists of reacting the appropriate N-acyl substituted aminobenzoic acids with Et chloroformate followed by further reaction with ammonia or a primary amine. Thus, e.g., to N-valeryl-5-iodoanthranilic acid in DMF is added Et3N and Et chloroformate; the reaction mixture is heated to 2 h until the evolution of carbon dioxide ceases, and then concentrated ammonium hydroxide is added; workup afforded 56.7% 2-Butyl-6-iodo-4-(3H)-quinazolinone.

RX(1) OF 1      A    ==>   B



RX(1)      RCT   A 158591-92-5

STAGE(1)

RGF   C 121-44-8 Et3N, D 541-41-3 ClCO2Et  
SOL   68-12-2 DMF

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STAGE(2)

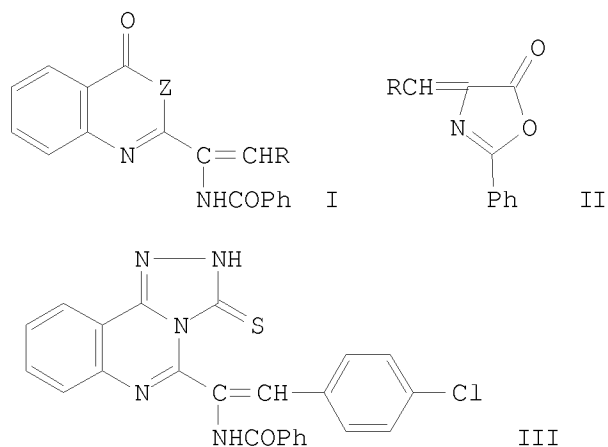
RGT E 1336-21-6 NH4OH

SOL 7732-18-5 Water

PRO B 143945-48-6

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

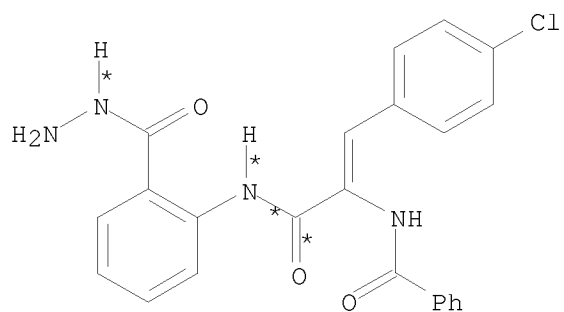
L3 ANSWER 133 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 121:35482 CASREACT  
TITLE: Synthesis and reactions of substituted benzoxazinones bearing a bulky group at position 2  
AUTHOR(S): Soliman, F. M. A.; Souka, L. M.; Eslam, I. E.; Dawood, N. T. A.  
CORPORATE SOURCE: Fac. Sci., Al-Azhar Univ., Cairo, Egypt  
SOURCE: Revue Roumaine de Chimie (1992), 37(10), 1153-8  
CODEN: RRCHAX; ISSN: 0035-3930  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB 2-Substituted 3,1-benzoxazin-4-ones I (Z = O, R = Ph or substituted phenyl) were prepared by reaction of oxazolones II with anthranilic acid. Reactions of I with amines and sodium azides were carried out. Thus, treatment of I (Z = O, R = p-ClC6H4) with H2NOH.HCl or semicarbazide gave quinazolone I (Z = N, R = p-ClC6H4) and triazole III, resp.

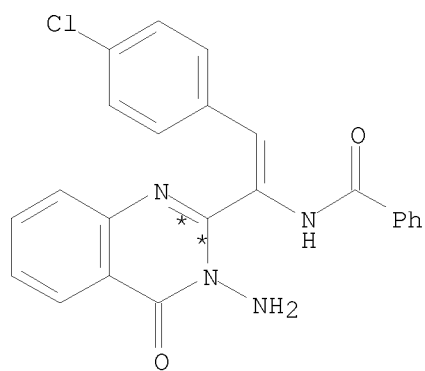
RX(18) OF 52 ...AC ==> AH

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AC

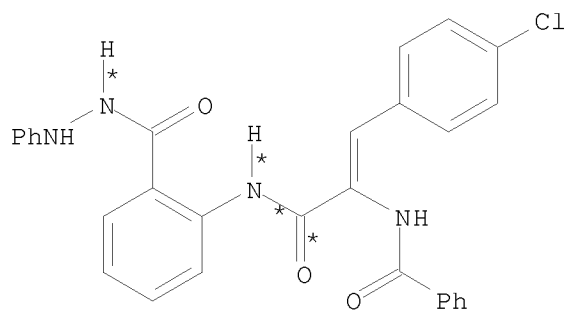
(18)  $\longrightarrow$



AH

RX(18)      RCT    AC 132994-54-8  
                  PRO    AH 132994-59-3

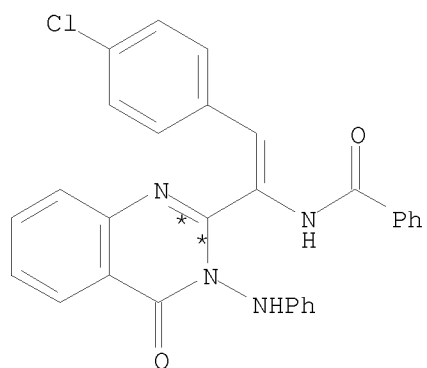
RX(19) OF 52      ...AE    ==>    AI



AE

(19)  $\longrightarrow$

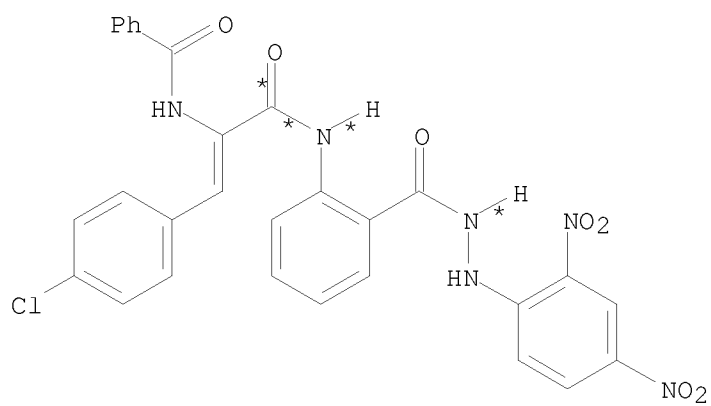
10/ 562,112



AI

RX(19)      RCT    AE 132994-55-9  
              PRO    AI 142075-10-3

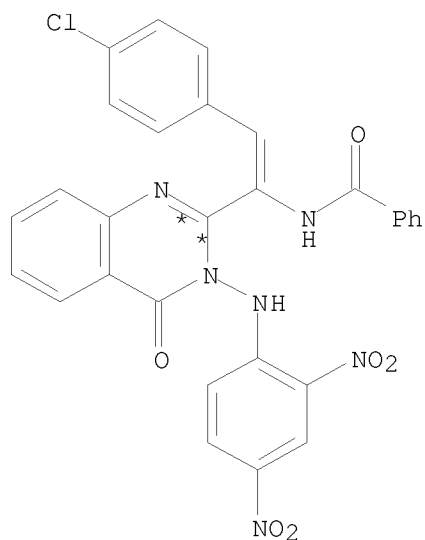
RX(20) OF 52      ...AG    ==>    AJ



AG

(20)  
→

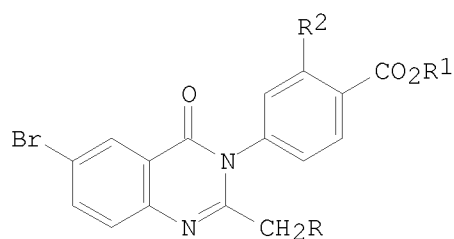
10/ 562,112



AJ

RX(20) RCT AG 141264-77-9  
PRO AJ 142075-11-4

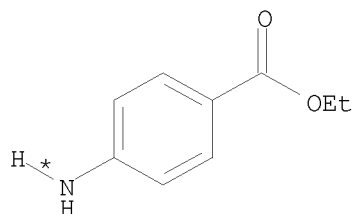
L3 ANSWER 134 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 120:323466 CASREACT  
TITLE: Synthesis and biological activities of  
6-bromo-2,3-disubstituted-4-(3H)-quinazolinones  
AUTHOR(S): Abdel-Alim, Abdel-Alim M.; El-Shorbagi, Abdel-Nasser  
A.; El-Shareif, Hosny A. H.; El-Gendy, Mahmoud A.;  
Amin, Monir A.  
CORPORATE SOURCE: Fac. Pharm., Assiut Univ., Cairo, Egypt  
SOURCE: Indian Journal of Chemistry, Section B: Organic  
Chemistry Including Medicinal Chemistry (1994),  
33B(3), 260-5  
CODEN: IJSBDB; ISSN: 0376-4699  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



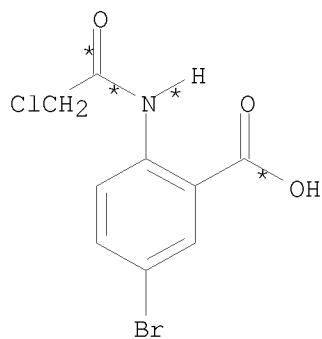
I

AB The title compds., 6-bromo-2, 3-disubstituted-4(3H)-quinazolinones (I) have been synthesized for evaluation as potential sedative-hypnotic, anti-convulsant and anti-inflammatory agents. Compound I (R = PhCH<sub>2</sub>S, R<sub>1</sub> = Et, R<sub>2</sub> = H) has been synthesized by condensing 6-bromo-2-chloromethyl-3-(p-ethoxycarbonylphenyl)-4(3H)-quinazolinone with benzyl mercaptan in the presence of potassium carbonate. Compds. I (R = CH<sub>2</sub>SCH<sub>2</sub>CO<sub>2</sub>H, CH<sub>2</sub>SCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H, CH<sub>2</sub>SCHMeCO<sub>2</sub>H) (II) are obtained by the condensation of I (R = Cl) with the appropriate thioacid. Superior sedative-hypnotic and anti-convulsant effects are achieved by II (R<sub>1</sub> = Me, Et; R<sub>2</sub> = H) (III). On the other hand, II (R<sub>2</sub> = OH) reveal better results as anti-inflammatory agents than that for III. Most of the tested compds. have been found to be, at least, two times as potent as aspirin in anti-inflammatory tests.

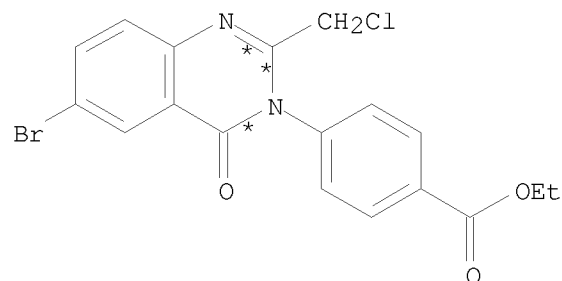
RX(1) OF 1 A + B ==> C



A



B

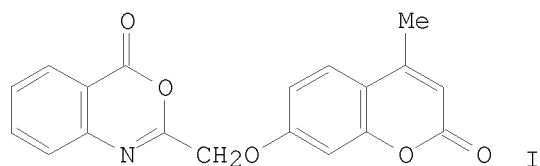


C  
YIELD 72%

RX(1) RCT A 94-09-7, B 155104-20-4  
RGT D 7719-12-2 PC13  
PRO C 155104-08-8  
SOL 1330-20-7 Xylene

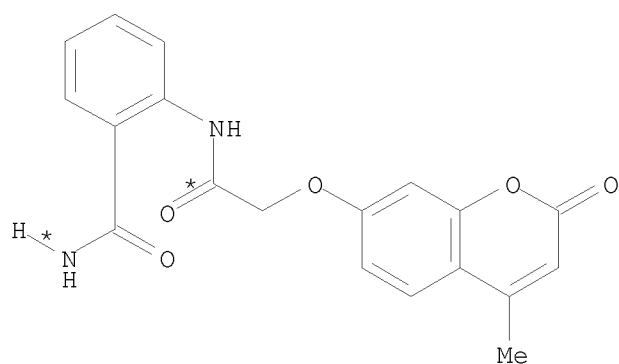
L3 ANSWER 135 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 120:323426 CASREACT  
TITLE: Synthesis and reactions of  
2-[[[4-methyl-2-oxo-2H-[1]benzopyran-7-yl]oxy]methyl]-

4H-3,1-benzoxazin-4-one  
 AUTHOR(S): Soliman, A. Y.; El-Assy, N. B.; El-Shahed, F.;  
 El-Kady, M.; El-Deen, I. M.  
 CORPORATE SOURCE: Fac. Sci, Ain Shams Univ., Egypt  
 SOURCE: Revue Roumaine de Chimie (1993), 38(1), 83-9  
 CODEN: RRCHAX; ISSN: 0035-3930  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB The relative reactivities of the  $\alpha$ -pyrone and oxazinone rings in I (title compound) with nucleophiles (Friedel-Crafts arylation, aminolysis, and hydrazinolysis) and electrophiles (aromatic aldehydes) are compared.

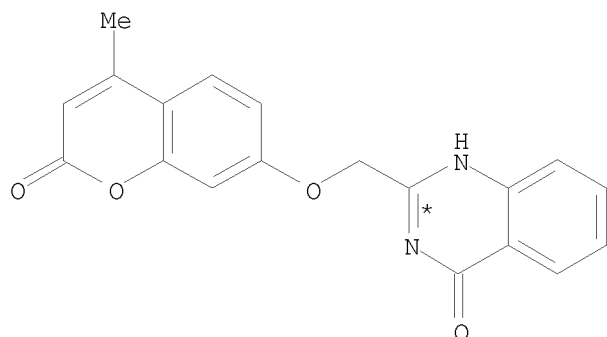
RX(15) OF 67 ...AC ==> AD



AC

(15)  $\longrightarrow$

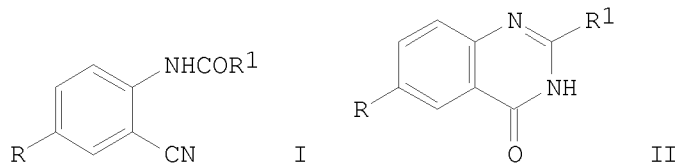
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AD  
YIELD 65%

RX(15)      RCT    AC 128649-83-2  
             RGT    AE 108-24-7 Ac2O  
             PRO    AD 128649-84-3

L3    ANSWER 136 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER:      120:217532    CASREACT  
TITLE:                    A facile preparation of quinazolin-4(3H)-ones from  
                             o-amido benzonitriles using sodium perborate  
AUTHOR(S):                Baudoin, Bernard; Ribeill, Yves; Vicker, Nigel  
CORPORATE SOURCE:        Dagenham Res. Cent., Rhone-Poulenc Rorer Ltd.,  
                             Dagenham/Essex, RM10 7XS, UK  
SOURCE:                    Synthetic Communications (1993), 23(20), 2833-7  
                             CODEN: SYNCAV; ISSN: 0039-7911  
DOCUMENT TYPE:            Journal  
LANGUAGE:                  English  
GI

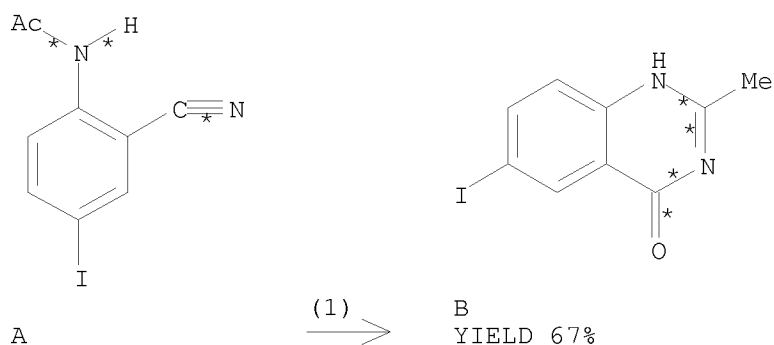


AB    The oxidation of o-amidobenzonitriles I (R = iodo, R1 = Me, ethylcyclohexyl;  
R = H, R1 = Ph; R = 3,4,5-trimethoxystyryl, R1 = Me2N, ethylcyclohexyl)  
using sodium perborate followed by cyclization afforded  
quinazolin-4(3H)-ones II in a one-pot reaction under mild, non-hazardous  
conditions.

RX(1) OF 1      A    ==>    B

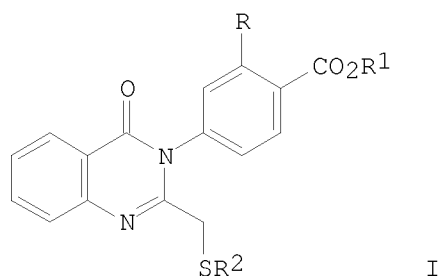


10/ 562,112



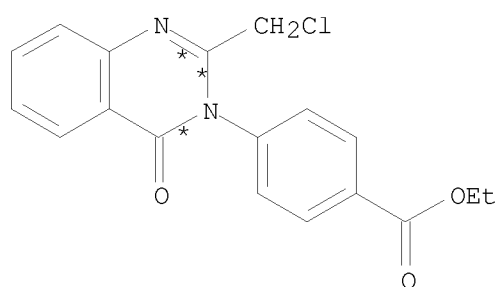
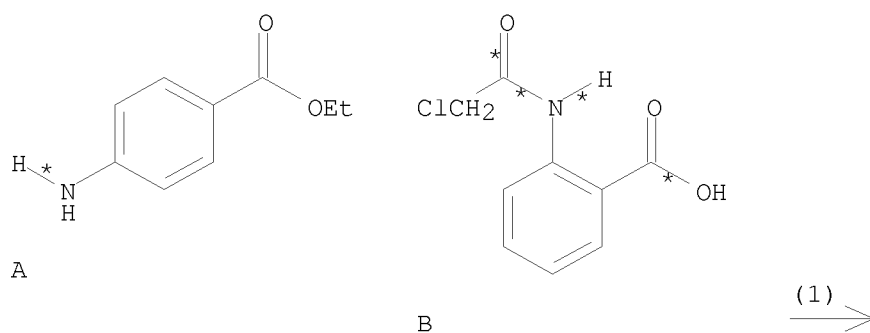
RX(1) RCT A 153861-34-8  
RGT C 7632-04-4 NaBO<sub>3</sub>  
PRO B 90347-75-4  
SOL 7732-18-5 Water, 123-91-1 Dioxane

L3 ANSWER 137 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 120:217521 CASREACT  
TITLE: Quinazolinone derivatives of biological interest. V.  
Novel 4(3H)-quinazolinones with sedative-hypnotic,  
anticonvulsant and antiinflammatory activities  
AUTHOR(S): Abdel-Alim, Abdel-Alim M.; El-Shorbagi, Nasser A.;  
El-Gendy, Mahmoud A.; El-Shareif, Hosny A. H.  
CORPORATE SOURCE: Pharm. Chem. Dep., Assiut Univ., Assiut, Egypt  
SOURCE: Collection of Czechoslovak Chemical Communications  
(1993), 58(8), 1963-8  
CODEN: CCCCAK; ISSN: 0010-0765  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB The title compds., I (R = H, HO; R<sub>1</sub> = alkyl; R<sub>2</sub> = Ph, benzyl, carboxyalkyl, etc.) and derivs. thereof were prepared. Their pharmacol. activity data for I as sedatives, hypnotics, anticonvulsants and inflammation inhibitors, analgesics, or antipyretics were not reported.

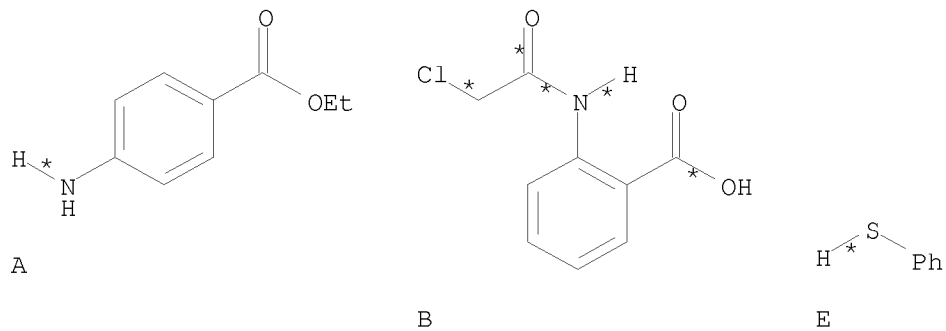
RX(1) OF 17 A + B ==> C...



C  
YIELD 76%

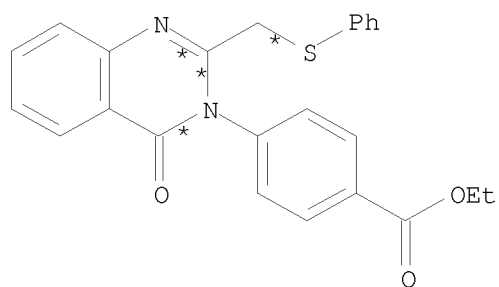
RX(1)      RCT    A 94-09-7, B 14422-49-2  
              RGT    D 7719-12-2 PC13  
              PRO    C 76535-04-1

RX(10) OF 17 COMPOSED OF RX(1), RX(2)  
 RX(10)      A + B + E  $\implies$  F



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2  
STEPS  
→

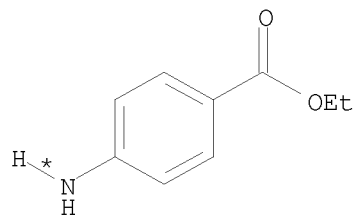


F  
YIELD 79%

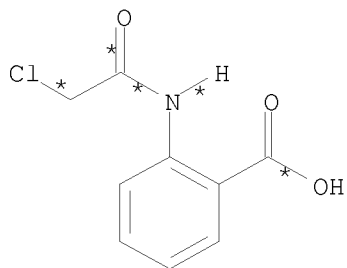
RX(1)      RCT    A 94-09-7, B 14422-49-2  
             RGT    D 7719-12-2 PC13  
             PRO    C 76535-04-1

RX(2)      RCT    E 108-98-5, C 76535-04-1  
             PRO    F 153705-92-1

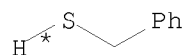
RX(11) OF 17 COMPOSED OF RX(1), RX(3)  
RX(11)      A + B + G ==> H



A



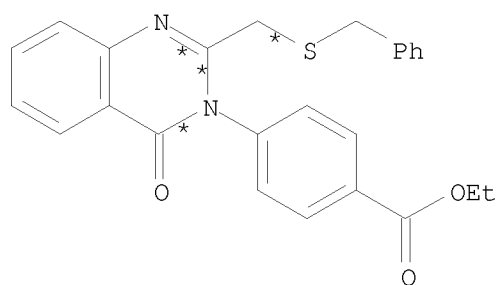
B



G

2  
STEPS  
→

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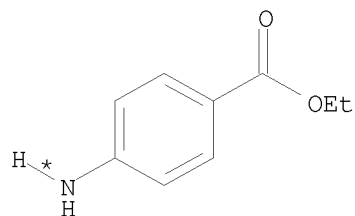


H  
YIELD 81%

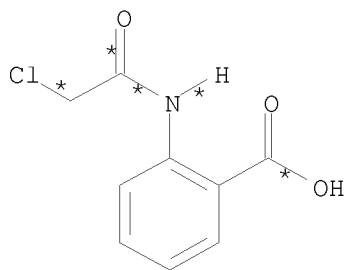
RX(1) RCT A 94-09-7, B 14422-49-2  
RGT D 7719-12-2 PC13  
PRO C 76535-04-1

RX(3) RCT G 100-53-8, C 76535-04-1  
PRO H 153705-94-3

RX(12) OF 17 COMPOSED OF RX(1), RX(4)  
RX(12) A + B + I ==> J



A



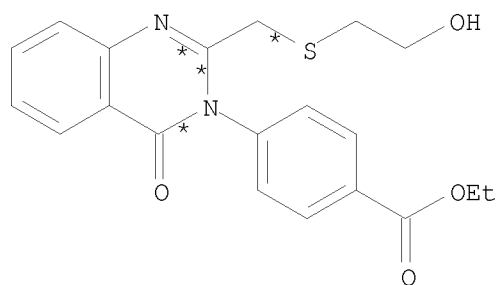
B



I

2  
STEPS  
→

10/ 562,112

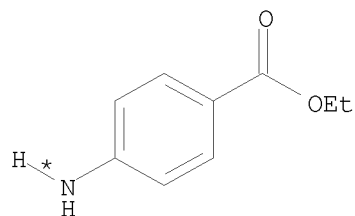


J  
YIELD 75%

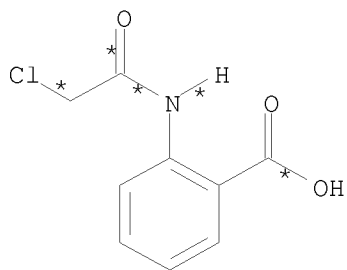
RX(1) RCT A 94-09-7, B 14422-49-2  
RGT D 7719-12-2 PC13  
PRO C 76535-04-1

RX(4) RCT I 60-24-2, C 76535-04-1  
PRO J 153705-98-7

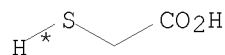
RX(13) OF 17 COMPOSED OF RX(1), RX(5)  
RX(13) A + B + K ==> L



A



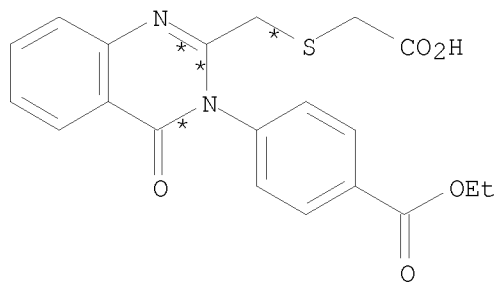
B



K

2  
STEPS  
→

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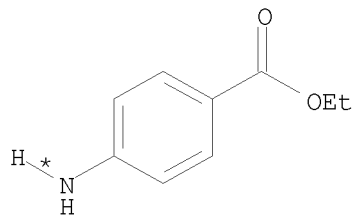


L  
YIELD 78%

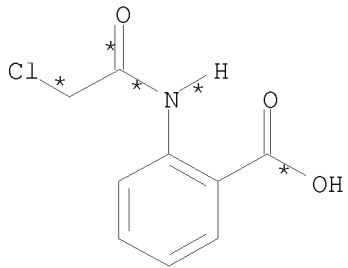
RX(1)      RCT    A 94-09-7, B 14422-49-2  
              RGT    D 7719-12-2 PC13  
              PRO    C 76535-04-1

RX(5) RCT K 68-11-1, C 76535-04-1  
PRO L 137731-84-1

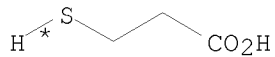
RX(14) OF 17 COMPOSED OF RX(1), RX(6)  
 RX(14) A + B + M ==> N



A



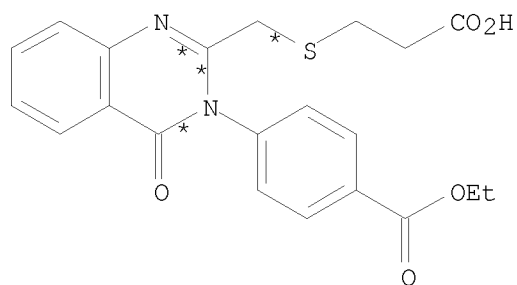
B



M

2  
STEPS  
→

10/ 562,112

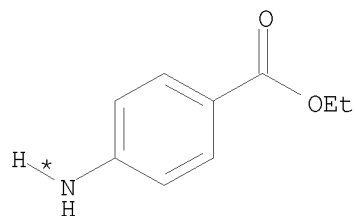


N  
YIELD 81%

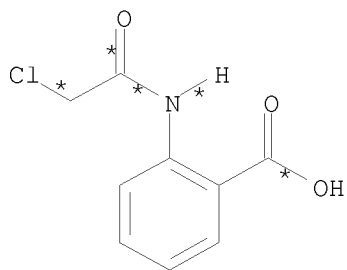
RX(1) RCT A 94-09-7, B 14422-49-2  
RGT D 7719-12-2 PC13  
PRO C 76535-04-1

RX(6) RCT M 107-96-0, C 76535-04-1  
PRO N 137731-85-2

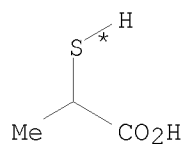
RX(15) OF 17 COMPOSED OF RX(1), RX(7)  
RX(15) A + B + O ==> P



A



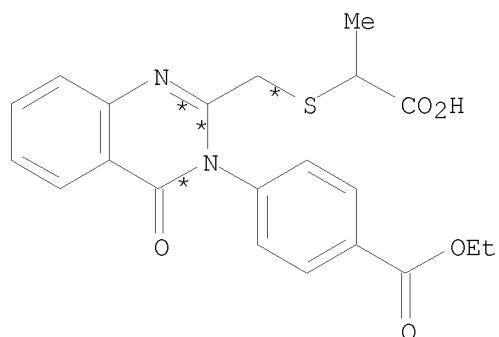
B



O

2  
STEPS  
→

10/ 562,112

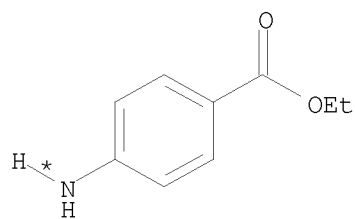


P  
YIELD 69%

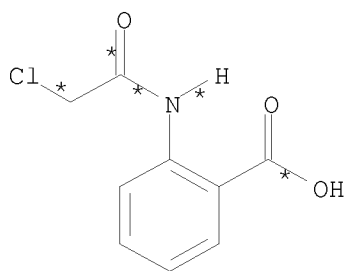
RX(1)      RCT    A 94-09-7, B 14422-49-2  
              RGT    D 7719-12-2 PC13  
              PRO    C 76535-04-1

RX(7)      RCT    O 79-42-5, C 76535-04-1  
              PRO    P 137731-86-3

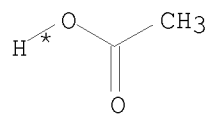
RX(16) OF 17 COMPOSED OF RX(1), RX(8)  
RX(16)      A + B + Q ==> R



A



B



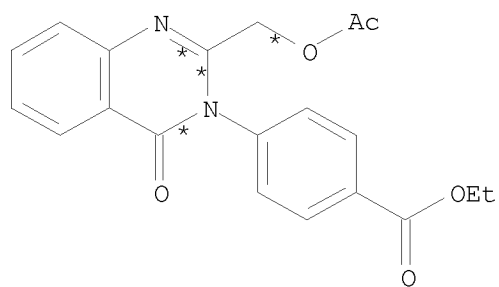
● Ag(I)

Q

2  
STEPS  
→



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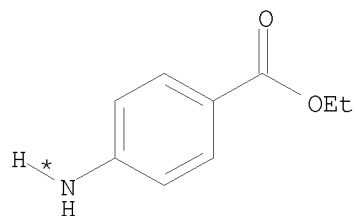


R  
YIELD 82%

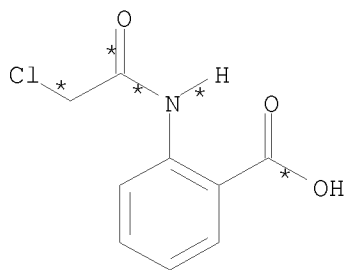
RX(1) RCT A 94-09-7, B 14422-49-2  
RGT D 7719-12-2 PC13  
PRO C 76535-04-1

RX(8) RCT Q 563-63-3, C 76535-04-1  
PRO R 153705-99-8

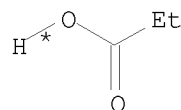
RX(17) OF 17 COMPOSED OF RX(1), RX(9)  
RX(17) A + B + S ==> T



A



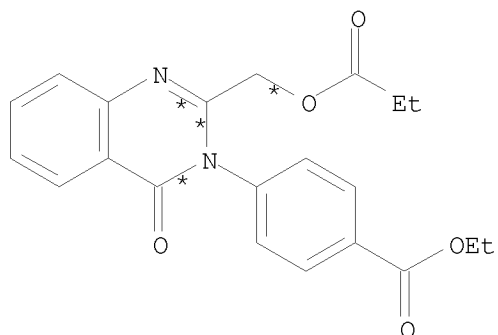
B



● Ag(I)

S

2  
STEPS  
→



T  
YIELD 83%

RX(1) RCT A 94-09-7, B 14422-49-2  
RGT D 7719-12-2 PC13  
PRO C 76535-04-1

RX(9) RCT S 5489-14-5, C 76535-04-1  
PRO T 153706-01-5

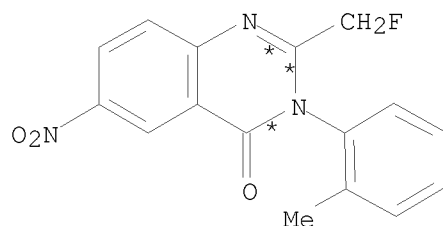
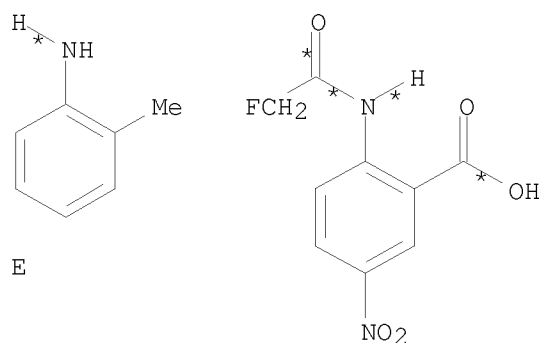
L3 ANSWER 138 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 119:139264 CASREACT  
TITLE: Preparation of 2-fluoroacetamido-5-nitrobenzoic acid  
and quinazoline derivative as intermediates for  
afloqualone  
INVENTOR(S): Kamifuji, Tamiro; Okatake, Mitsuru  
PATENT ASSIGNEE(S): Sumika Fuain Kemu KK, Japan; Sumika Fine Chemicals  
Co., Ltd.  
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05097788	A	19930420	JP 1991-283651	19911002
JP 2816778	B2	19981027		

PRIORITY APPLN. INFO.: JP 1991-283651 19911002

AB 2-Fluoromethyl-3-(2-methylphenyl)-6-nitro-4(3H)quinazolinone (I) is prepared by treatment of 5-nitroanthranilic acid (II) suspended in organic solvents with monofluoroacetyl chloride (III), followed by treatment of resulting 2-fluoroacetamido-5-nitrobenzoic acid (IV) with o-toluidine (V). Treatment of II with III in MeCN at .apprx.40° for 3-5 h gave 97.5% IV, which was treated with PC13 and V in CH2Cl2 at .apprx.40° for 9 h to afford 93.8% I.

RX(2) OF 3 ...E + C ==> F



F  
YIELD 93%

RX(2)      RCT    E 95-53-4, C 87266-10-2  
              RGT    G 7719-12-2 PC13  
              PRO    F 56287-73-1  
              SOL    75-09-2 CH2Cl2

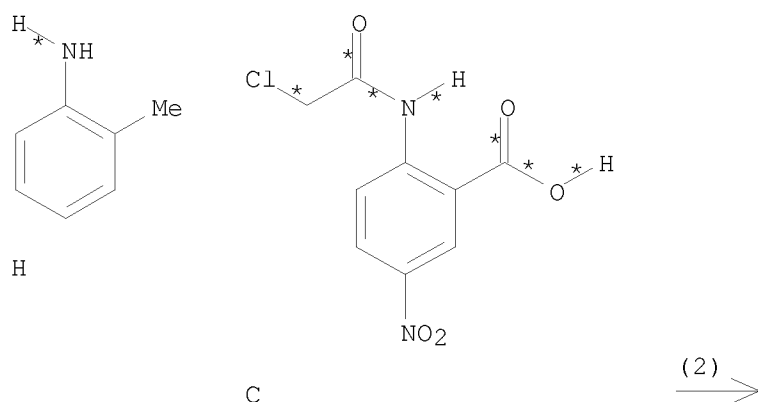
L3    ANSWER 139 OF 258    CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER:      119:95552 CASREACT  
 TITLE:                    Preparation of quinazolinone derivative as an  
                                  intermediate for afloqualone  
 INVENTOR(S):            Kamifuji, Tamiro; Matsui, Kozo; Okatake, Mitsuru  
 PATENT ASSIGNEE(S):    Sumika Fuain Kemu Kk, Japan  
 SOURCE:                   Jpn. Kokai Tokkyo Koho, 4 pp.  
                                  CODEN: JKXXAF  
 DOCUMENT TYPE:        Patent  
 LANGUAGE:               Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05078333	A	19930330	JP 1991-86166	19910325
JP 2761677	B2	19980604		
PRIORITY APPLN. INFO.:			JP 1991-86166	19910325

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AB 2-Fluoromethyl-3-(2-methylphenyl)-6-nitro-4(3H)-quinazolinone (I), useful as an intermediate for minor tranquilizing and muscle relaxing afloqualone, is prepared by treatment of 2-fluoroacetamido-5-nitrobenzoic acid (II) with o-toluidine. Treatment of 5-nitroanthranilic acid with AcNH<sub>2</sub>, Me<sub>3</sub>SiCl, and Et<sub>3</sub>N in CH<sub>2</sub>Cl<sub>2</sub> at .apprx.42° for 1 h, then with monofluoroacetyl chloride at .apprx.42° for 3 h gave 98.2% II, which was treated with o-toluidine and PCl<sub>3</sub> in CH<sub>2</sub>Cl<sub>2</sub> at .apprx.40° for 9 h to afford 93.8% I.

RX(2) OF 3 ...H + C ==> I



I  
YIELD 93%

RX(2) RCT H 95-53-4, C 135590-27-1  
RGT J 7719-12-2 PCl<sub>3</sub>  
PRO I 56287-73-1  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

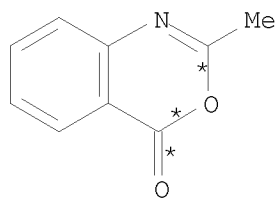
L3 ANSWER 140 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 117:69816 CASREACT  
TITLE: Synthesis and some reactions of aryl pyridyl sulfide derivatives

AUTHOR(S): Abbady, M. S.  
 CORPORATE SOURCE: Fac. Sci., Assiut Univ., Assiut, Egypt  
 SOURCE: Phosphorus, Sulfur and Silicon and the Related  
 Elements (1992), 68(1-4), 69-76  
 CODEN: PSSLEC; ISSN: 1042-6507  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

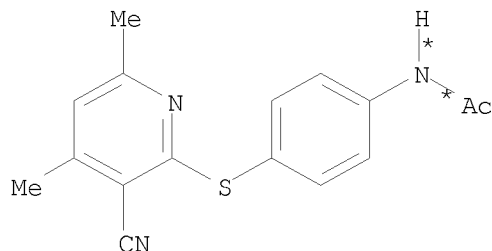
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Aminophenylthiopyridine I (R = NH<sub>2</sub>) (II) was prepared by reaction of 2-chloro-3-cyano-4,6-dimethylpyridine and 4-bromonitrobenzene in aqueous sodium sulfide solution. Condensation of II with aromatic aldehydes, 2-methylbenzoxazin-4-one, azalactone and succinic anhydride afforded the expected products I (R = N:CHC<sub>6</sub>H<sub>4</sub>R<sub>1</sub>, Q, Q1, Q2; R<sub>1</sub> = H, 4-NO<sub>2</sub>, 4-NMe<sub>2</sub>, 2-OH). Coupling of I (R = N:NC1) with active methylene compds. gave the corresponding hydrazones I (R = NHN:CR<sub>2</sub>CO<sub>2</sub>Et, R<sub>2</sub> = Ac, cyano). Cyclization of I (R = NHN:CAcCO<sub>2</sub>Et) with AlCl<sub>3</sub> gave the cinnoline derivative III which condensed with phenylhydrazine to give the pyrazolocinnoline derivative IV. Oxidation of some of the prepared sulfides with H<sub>2</sub>O<sub>2</sub> in AcOH afforded the corresponding sulfones.

RX(9) OF 58 ...R + F ==> S...



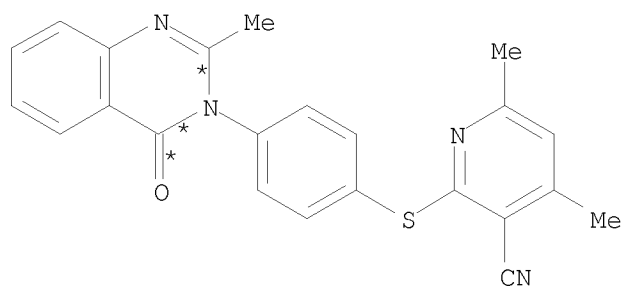
R



F



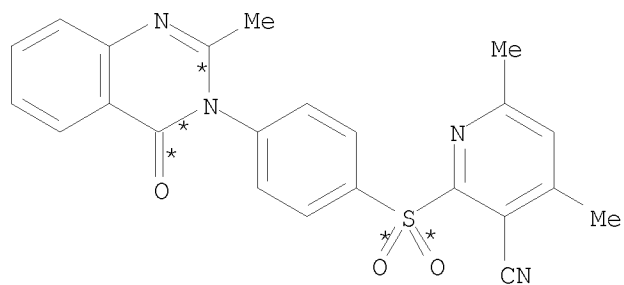
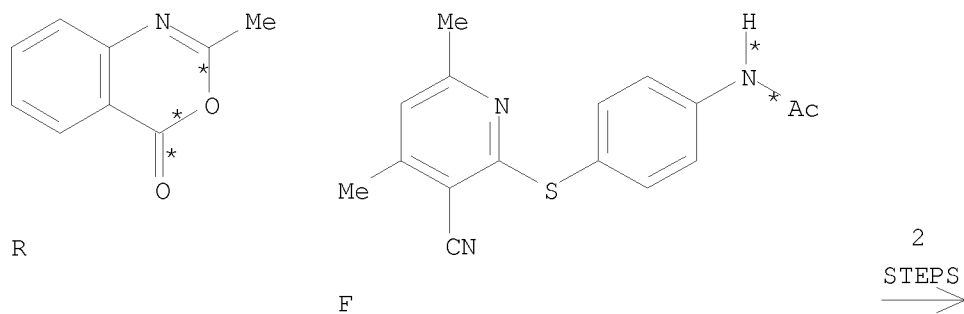
10/ 562,112



S  
YIELD 58%

RX(9) RCT R 525-76-8, F 142531-61-1  
PRO S 142531-65-5

RX(36) OF 58 COMPOSED OF RX(9), RX(10)  
RX(36) R + F ==> T



T  
YIELD 42%

RX(9) RCT R 525-76-8, F 142531-61-1  
PRO S 142531-65-5

RX(10) RCT S 142531-65-5

RGT H 7722-84-1 H2O2  
PRO T 142531-66-6

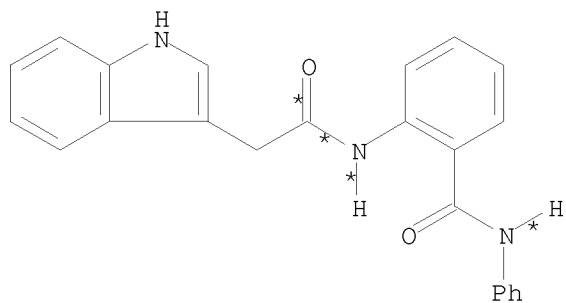
L3 ANSWER 141 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 117:69809 CASREACT  
TITLE: Synthesis and x-ray crystallographic analysis of  
quinazolinone cholecystokinin/gastrin receptor ligands  
AUTHOR(S): Yu, Melvin J.; McCowan, Jefferson R.; Mason, Norman  
R.; Deeter, Jack B.; Mendelsohn, Laurane G.  
CORPORATE SOURCE: Lilly Res. Lab., Eli Lilly Co., Indianapolis, IN,  
46285, USA  
SOURCE: Journal of Medicinal Chemistry (1992), 35(14), 2534-42  
CODEN: JMCMAR; ISSN: 0022-2623  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Compds. exemplified by 4(3H)-quinazolinone I (X = OCHMe2, Y = Br, n = 2) (II) (IC50 = 0.0093  $\mu$ M using mouse brain membranes) represent a structurally novel series of non-peptide cholecystokinin B receptor ligands. Since asperlicin, a selective CCK-A receptor antagonist, may be regarded as a conformationally constrained 2-substituted-3-phenyl-4(3H)-quinazolinone, the progenitor of compound II, compound I (X = Y = H, n = 2), might therefore represent a conformationally flexible pharmacophore of the natural product. Quinazolinone derivs., e.g. I (X = Y = H; n = 1, 2, 3), III and IV (R = H, Me), were prepared in order to probe possible conformational preferences for this class of receptor ligands, in particular the spatial relationship between the indole and quinazolinone rings. Thus, anilide V was treated with 1,3-dioxane-4,6-dione VI in the presence of pyridium tosylate in pyridine to give IV (R = H). The x-ray crystal structure conformation for IV (R = H) (IC50 = 0.026  $\mu$ M) is extended with the two heteroarom. rings adopting an antiperiplanar arrangement around the central  $\sigma$  bond of the ethane linker, whereas the solid-state conformation for a less active analog III (IC50 = 9.1  $\mu$ M) is folded with the two heteroarom. systems adopting a synclinal orientation. However, MM2 force field calcns. (MacroModel, v 3.0) suggest that the energy difference between the folded and extended conformation is small and that other factors such as unfavorable steric interactions may account for the difference in receptor affinity. For derivs. with one or to three methylene units separating the indole and quinazolinone rings, maximal receptor binding activity was found when the distance separating the two heteroarom. systems is defined by an Et group. Introducing unsatn. into the ethylene bridge of II limited the conformational flexibility of the mol. and decreased its receptor affinity greater than 2 orders of magnitude.

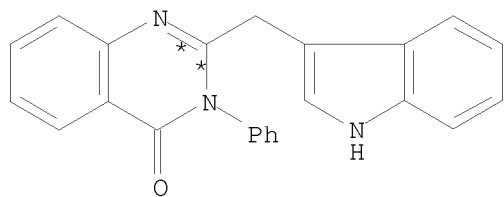
RX(2) OF 17 ...F ==> G

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F

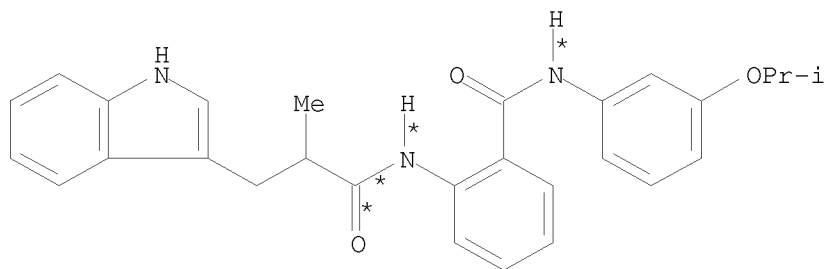
(2)  $\longrightarrow$



G

RX(2) RCT F 142005-24-1  
 RGT H 104-15-4 TsOH  
 PRO G 139571-49-6  
 SOL 108-88-3 PhMe  
 NTE Key step

RX(4) OF 17 ...L ==> O

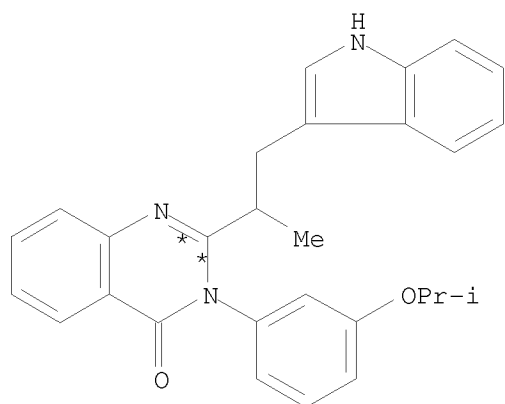


L

(4)  $\longrightarrow$



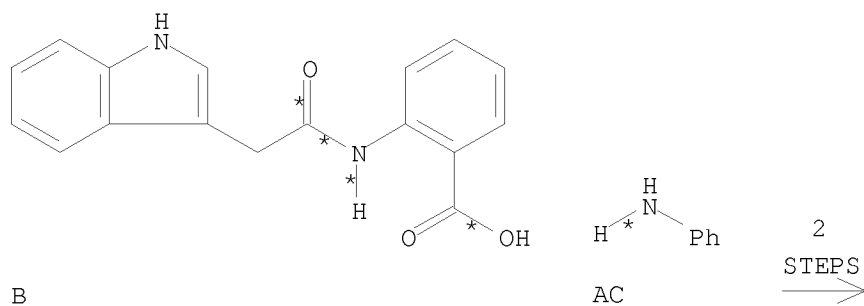
10/ 562,112



O

RX(4)      RCT    L 142005-17-2  
              RGT    P 24057-28-1 Pyridinium tosylate  
              PRO    O 142005-18-3  
              SOL    110-86-1 Pyridine  
              NTE    Key step

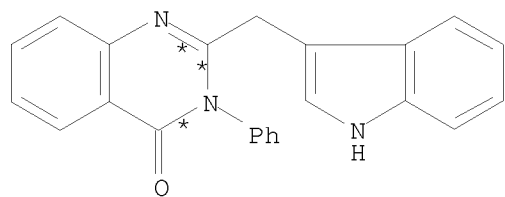
RX(14) OF 17 COMPOSED OF RX(9), RX(2)  
 RX(14)      B    +    AC    ==>    G



B

AC

2  
 STEPS  
 →



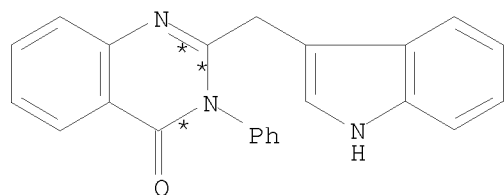
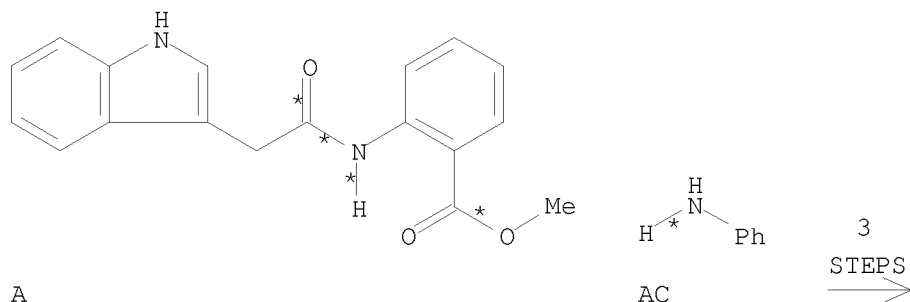
G

RX(9)      RCT    B 57932-49-7, AC 62-53-3  
              RGT    M 530-62-1 Diimidazolyl ketone, P 24057-28-1 Pyridinium tosylate  
              PRO    F 142005-24-1  
              SOL    109-99-9 THF

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RX(2)      RCT    F 142005-24-1  
             RGT    H 104-15-4 TsOH  
             PRO    G 139571-49-6  
             SOL    108-88-3 PhMe  
             NTE    Key step

RX(15) OF 17 COMPOSED OF RX(1), RX(9), RX(2)  
RX(15)      A    +    AC    ==>    G



RX(1)      RCT    A 139543-68-3  
             RGT    C 1310-73-2 NaOH  
             PRO    B 57932-49-7  
             SOL    7732-18-5 Water, 67-56-1 MeOH

RX(9)      RCT    B 57932-49-7, AC 62-53-3  
             RGT    M 530-62-1 Diimidazolyl ketone, P 24057-28-1 Pyridinium tosylate  
             PRO    F 142005-24-1  
             SOL    109-99-9 THF

RX(2)      RCT    F 142005-24-1  
             RGT    H 104-15-4 TsOH  
             PRO    G 139571-49-6  
             SOL    108-88-3 PhMe  
             NTE    Key step

TITLE: The synthesis of some 3-amino-2-(halomethyl)-, 2-(halomethyl)-3-(substituted amino)- and 2-(halomethyl)-3-hetarylquinazolin-4(3H)-ones as potential plant protecting agents

AUTHOR(S): Fetter, Jozsef; Czuppon, Tibor; Hornyak, Gyula; Feller, Antal

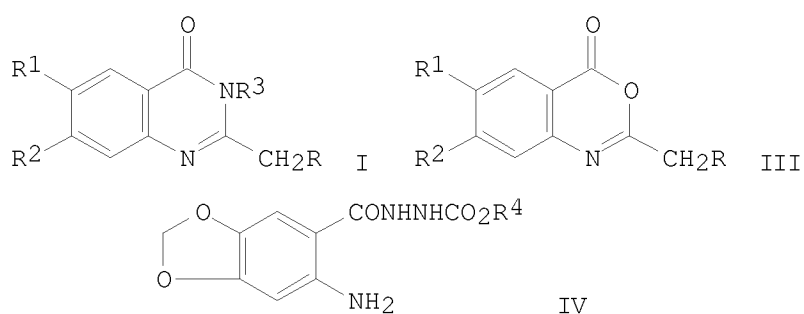
CORPORATE SOURCE: Dep. Org. Chem., Tech. Univ. Budapest, Budapest, H-1521, Hung.

SOURCE: Tetrahedron (1991), 47(45), 9393-410  
CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

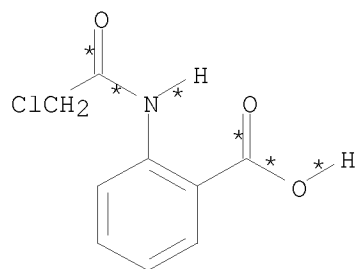
GI



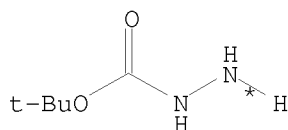
AB A series of quinazolinyl carbazates I [R = F, Cl, Br; R<sup>1</sup> = H, NO<sub>2</sub>; R<sup>2</sup> = H or R<sup>1</sup>R<sup>2</sup> = OCH<sub>2</sub>O; R<sup>3</sup> = NHCO<sub>2</sub>Et, NHCO<sub>2</sub>CMe<sub>3</sub> (II)] and hetaryl derivs. I (R<sup>1</sup> = 3,5-dimethyl-4-oxazolyl, 3,5-dimethyl-4-pyrazolyl) were obtained by reacting benzoxazinones III (R<sup>3</sup> = NHCO<sub>2</sub>CMe<sub>3</sub>) with alkyl carbazates and hetaryl amines, resp. Some of the carbazates II were obtained alternatively by treatment of carbazate IV (R<sup>4</sup> = Et, CMe<sub>3</sub>) with haloacetyl halides. The tert-Bu carbazates I (R<sup>3</sup> = NHCO<sub>2</sub>CMe<sub>3</sub>) were converted into amino quinazolinones I (R<sup>3</sup> = NH<sub>2</sub>), some of which were further converted into dimethylpyrrolyl derivs. I (R<sup>3</sup> = 2,5-dimethyl-1-pyrrolyl). I (R<sup>3</sup> = NH<sub>2</sub>; R<sup>2</sup> = R<sup>1</sup> = H; R = Br) was obtained by brominating its 2-Me analog with cyanogen bromide. Biol. screening showed that some of the prepared quinazolines, namely I (R<sup>3</sup> = NH<sub>2</sub>; R<sup>1</sup> = R<sup>2</sup> = H; R = Cl) had a significant antifungal activity, while I (R<sup>3</sup> = 3,5-dimethyl-4-pyrazolyl; R<sup>1</sup> = R<sup>2</sup> = H; R = F) had an effect on various functions of the CNS.

RX(53) OF 131 COMPOSED OF RX(7), RX(18)  
RX(53) C + T ==> AC

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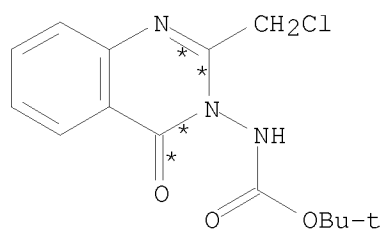


C



T

2  
STEPS  
→

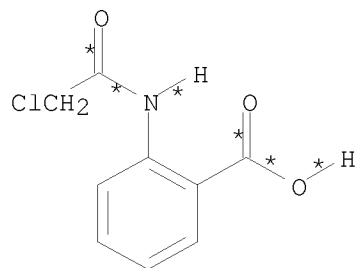


AC  
YIELD 80%

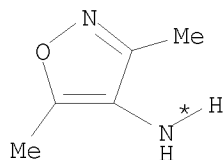
RX(7)      RCT    C 14422-49-2  
              RGT    M 108-24-7 Ac2O  
              PRO    L 98592-35-9

RX(18)      RCT    T 870-46-2, L 98592-35-9  
              PRO    AC 138639-39-1

RX(54) OF 131 COMPOSED OF RX(7), RX(36)  
RX(54)      C    +    AT    ==>    AU



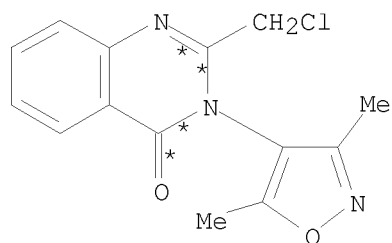
C



AT

2  
STEPS  
→

10/ 562,112

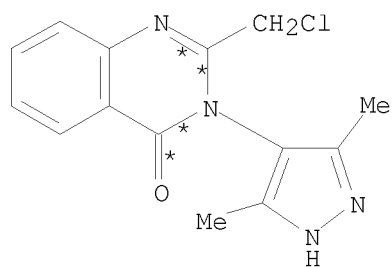
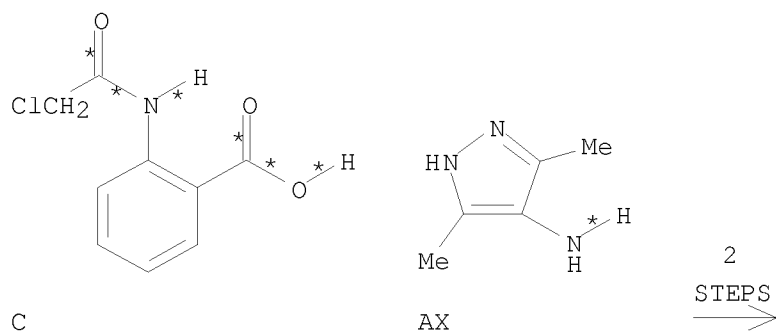


AU  
YIELD 67%

RX(7)        RCT   C 14422-49-2  
              RGT   M 108-24-7 Ac2O  
              PRO   L 98592-35-9

RX(36)       RCT   AT 31329-64-3, L 98592-35-9  
              PRO   AU 138639-52-8

RX(55) OF 131 COMPOSED OF RX(7), RX(39)  
RX(55)       C   +   AX   ==>   AY



AY  
YIELD 67%

RX(7)        RCT   C 14422-49-2  
              RGT   M 108-24-7 Ac2O

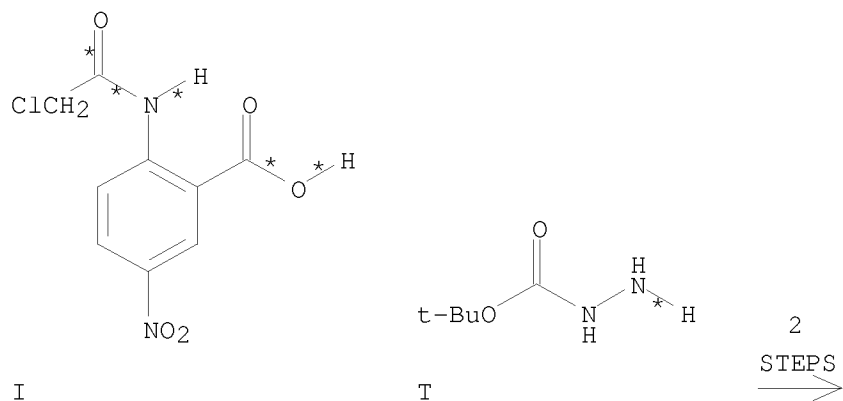
10/ 562,112

PRO L 98592-35-9

RX(39) RCT AX 5272-86-6, L 98592-35-9  
PRO AY 138639-56-2

RX(56) OF 131 COMPOSED OF RX(8), RX(19)

RX(56) I + T ==> AD



AD

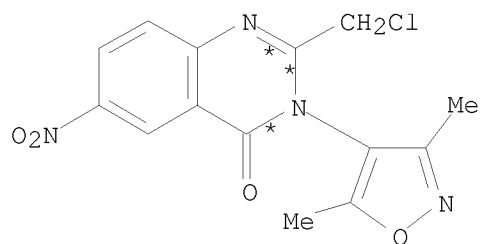
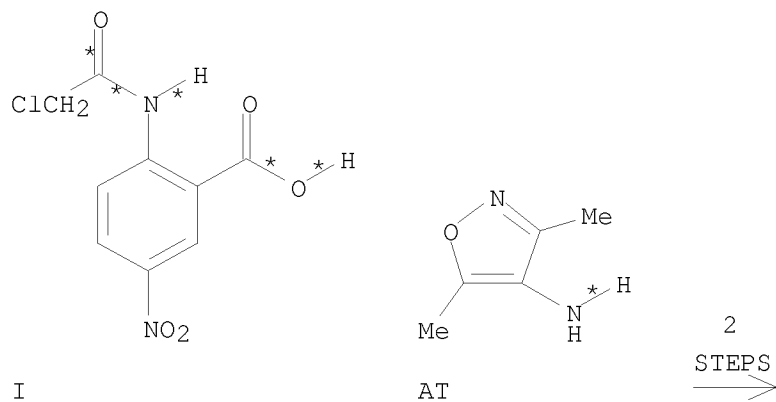
RX(8) RCT I 135590-27-1  
RGT M 108-24-7 Ac<sub>2</sub>O  
PRO N 138639-61-9

RX(19) RCT T 870-46-2, N 138639-61-9  
PRO AD 138639-41-5

RX(57) OF 131 COMPOSED OF RX(8), RX(37)

RX(57) I + AT ==> AV

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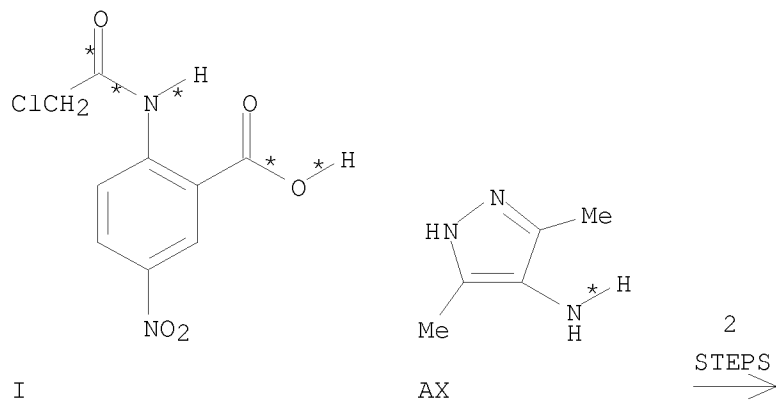


AV  
YIELD 72%

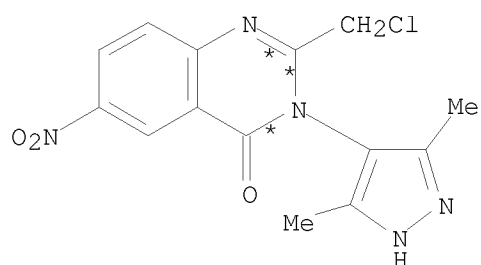
RX(8) RCT I 135590-27-1  
RGT M 108-24-7 Ac2O  
PRO N 138639-61-9

RX(37) RCT AT 31329-64-3, N 138639-61-9  
PRO AV 138639-53-9

RX(58) OF 131 COMPOSED OF RX(8), RX(40)  
RX(58) I + AX ==> AZ



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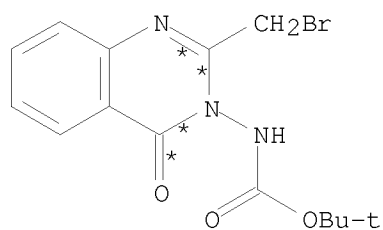
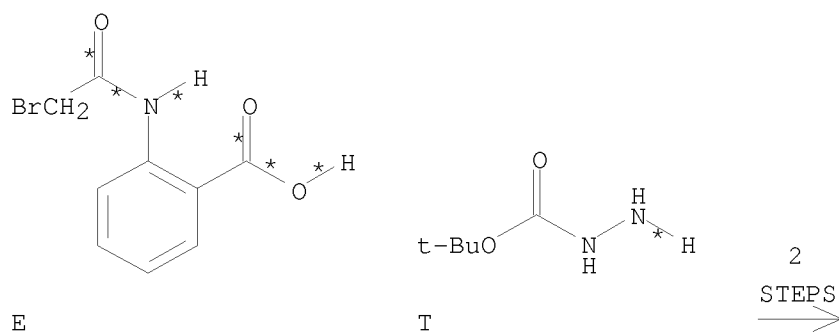


AZ  
YIELD 81%

RX(8)        RCT    I 135590-27-1  
              RGT    M 108-24-7 Ac2O  
              PRO    N 138639-61-9

RX(40)       RCT    AX 5272-86-6, N 138639-61-9  
              PRO    AZ 138639-58-4

RX(62) OF 131 COMPOSED OF RX(10), RX(22)  
RX(62)       E    +    T    ==>    AF



AF  
YIELD 51%

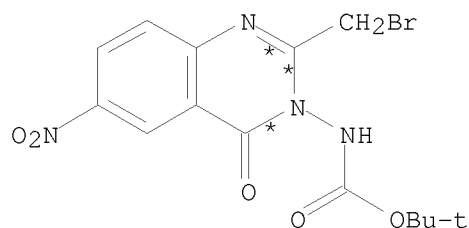
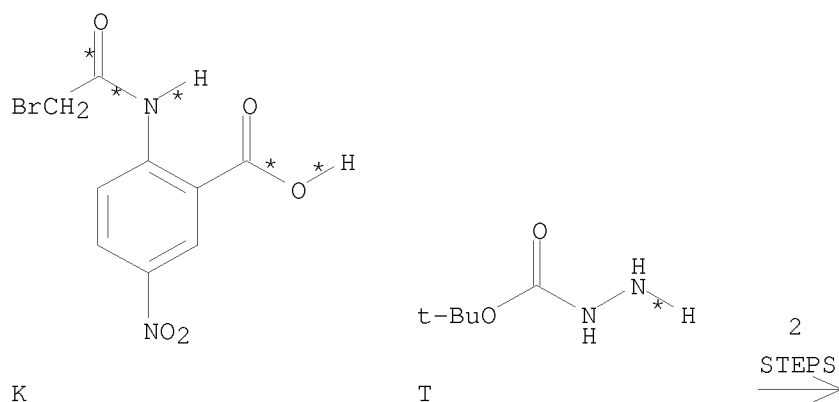


10/ 562,112

RX(10)      RCT   E 5979-85-1  
              RGT   M 108-24-7 Ac2O  
              PRO   P 43160-23-2

RX(22)      RCT   T 870-46-2, P 43160-23-2  
              PRO   AF 138639-40-4

RX(63) OF 131 COMPOSED OF RX(11), RX(25)  
RX(63)      K   +   T   ==>   AH



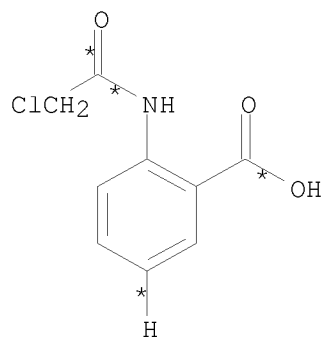
AH  
YIELD 55%

RX(11)      RCT   K 138639-68-6  
              RGT   M 108-24-7 Ac2O  
              PRO   Q 138639-62-0

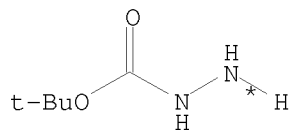
RX(25)      RCT   T 870-46-2, Q 138639-62-0  
              PRO   AH 138639-42-6

RX(92) OF 131 COMPOSED OF RX(5), RX(8), RX(19)  
RX(92)      C   +   T   ==>   AD

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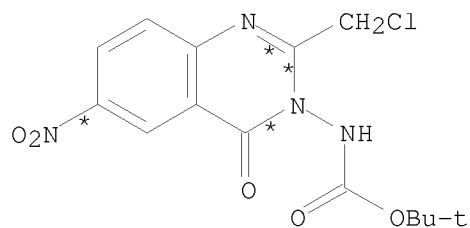


C



T

3  
STEPS  
→



AD

RX(5)      RCT    C 14422-49-2  
             RGT    J 7697-37-2 HNO3  
             PRO    I 135590-27-1

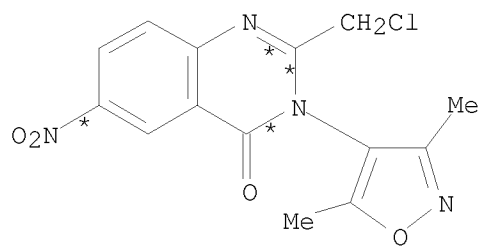
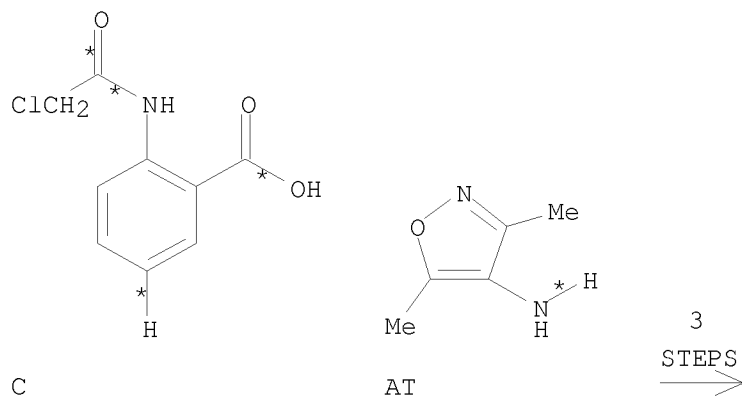
RX(8)      RCT    I 135590-27-1  
             RGT    M 108-24-7 Ac2O  
             PRO    N 138639-61-9

RX(19)     RCT    T 870-46-2, N 138639-61-9  
             PRO    AD 138639-41-5

RX(93) OF 131 COMPOSED OF RX(5), RX(8), RX(37)

RX(93)      C    +    AT    ==>    AV

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AV  
YIELD 72%

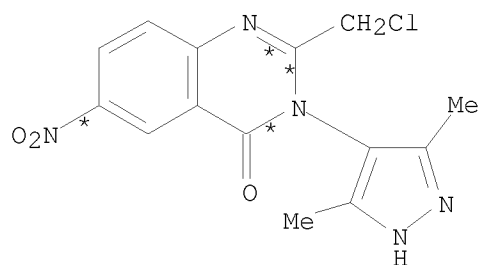
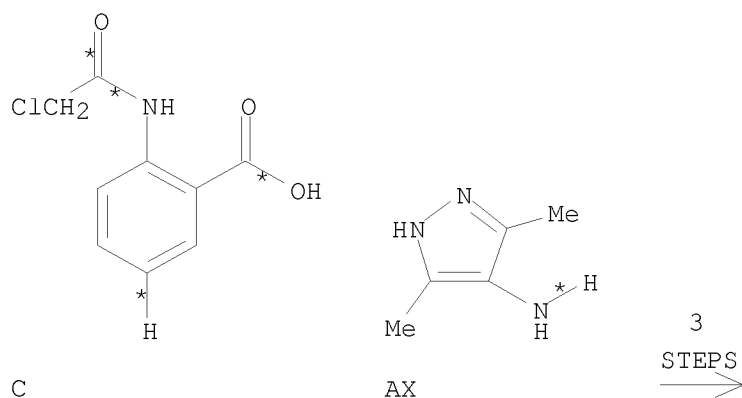
RX(5) RCT C 14422-49-2  
RGT J 7697-37-2 HNO3  
PRO I 135590-27-1

RX(8) RCT I 135590-27-1  
RGT M 108-24-7 Ac2O  
PRO N 138639-61-9

RX(37) RCT AT 31329-64-3, N 138639-61-9  
PRO AV 138639-53-9

RX(94) OF 131 COMPOSED OF RX(5), RX(8), RX(40)  
RX(94) C + AX ==> AZ

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AZ  
YIELD 81%

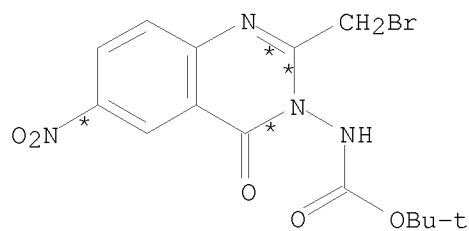
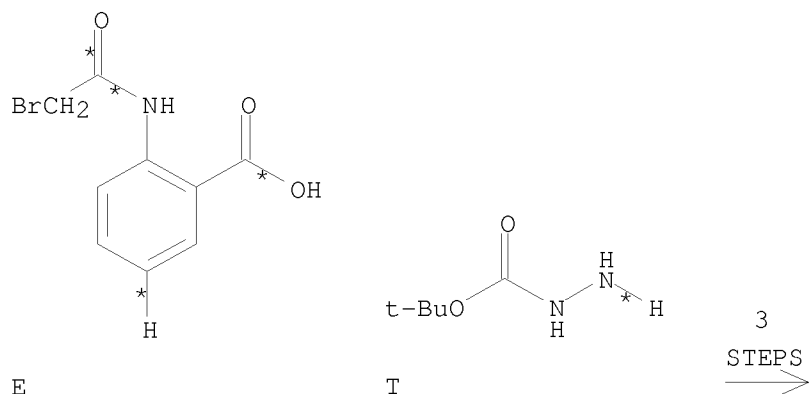
RX(5)      RCT    C 14422-49-2  
              RGT    J 7697-37-2 HNO3  
              PRO    I 135590-27-1

RX(8)      RCT    I 135590-27-1  
              RGT    M 108-24-7 Ac2O  
              PRO    N 138639-61-9

RX(40)     RCT    AX 5272-86-6, N 138639-61-9  
              PRO    AZ 138639-58-4

RX(98) OF 131 COMPOSED OF RX(6), RX(11), RX(25)  
 RX(98)      E    +    T    ==>    AH

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AH  
YIELD 55%

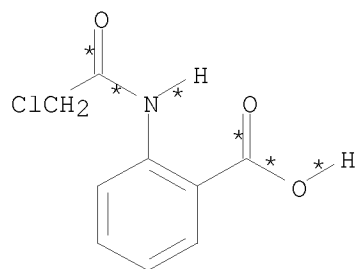
RX(6) RCT E 5979-85-1  
RGT J 7697-37-2 HNO3  
PRO K 138639-68-6

RX(11) RCT K 138639-68-6  
RGT M 108-24-7 Ac2O  
PRO Q 138639-62-0

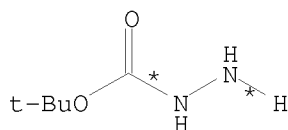
RX(25) RCT T 870-46-2, Q 138639-62-0  
PRO AH 138639-42-6

RX(100) OF 131 COMPOSED OF RX(7), RX(18), RX(26)  
RX(100) C + T ==> AI

10/ 562,112

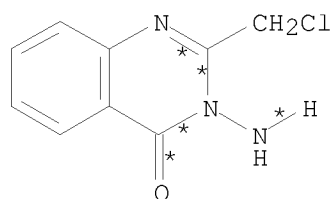


C



T

3  
STEPS  
→



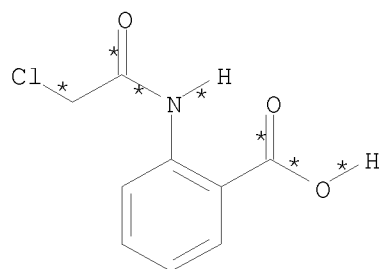
AI  
YIELD 70%

RX(7) RCT C 14422-49-2  
RGT M 108-24-7 Ac2O  
PRO L 98592-35-9

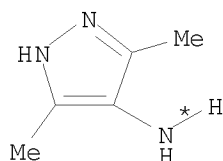
RX(18) RCT T 870-46-2, L 98592-35-9  
PRO AC 138639-39-1

RX(26) RCT AC 138639-39-1  
RGT AJ 64-19-7 AcOH  
PRO AI 138639-45-9

RX(101) OF 131 COMPOSED OF RX(7), RX(39), RX(44)  
RX(101) C + AX ==> BE



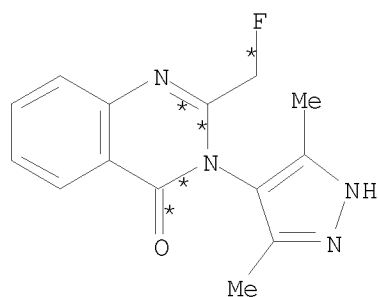
C



AX

3  
STEPS  
→

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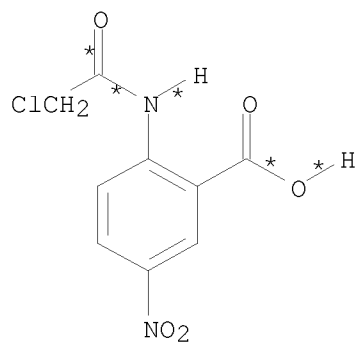
BE  
YIELD 31%

RX(7)        RCT    C 14422-49-2  
              RGT    M 108-24-7 Ac2O  
              PRO    L 98592-35-9

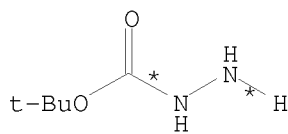
RX(39)       RCT    AX 5272-86-6, L 98592-35-9  
              PRO    AY 138639-56-2

RX(44)       RCT    AY 138639-56-2  
              RGT    BC 7789-23-3 KF  
              PRO    BE 138639-57-3

RX(104) OF 131 COMPOSED OF RX(8), RX(19), RX(29)  
RX(104)    I    +    T    ==>    AN



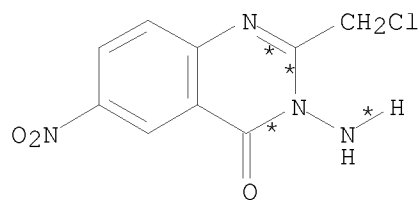
I



T

3  
STEPS  
=>

10/ 562,112



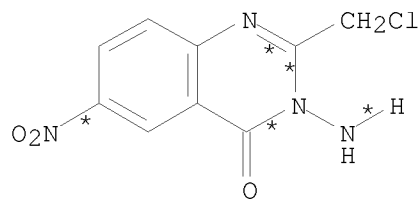
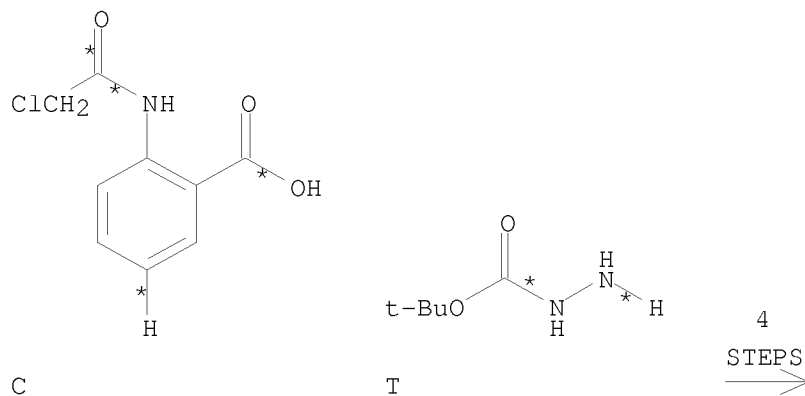
AN  
YIELD 57%

RX(8) RCT I 135590-27-1  
RGT M 108-24-7 Ac2O  
PRO N 138639-61-9

RX(19) RCT T 870-46-2, N 138639-61-9  
PRO AD 138639-41-5

RX(29) RCT AD 138639-41-5  
PRO AN 138639-46-0

RX(105) OF 131 COMPOSED OF RX(5), RX(8), RX(19), RX(29)  
RX(105) C + T ==> AN



AN  
YIELD 57%



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RX(5)        RCT    C 14422-49-2  
              RGT    J 7697-37-2 HNO3  
              PRO    I 135590-27-1

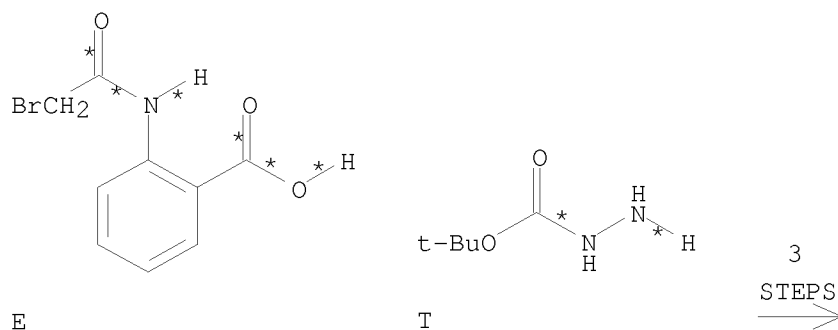
RX(8)        RCT    I 135590-27-1  
              RGT    M 108-24-7 Ac2O  
              PRO    N 138639-61-9

RX(19)       RCT    T 870-46-2, N 138639-61-9  
              PRO    AD 138639-41-5

RX(29)       RCT    AD 138639-41-5  
              PRO    AN 138639-46-0

RX(110) OF 131 COMPOSED OF RX(10), RX(22), RX(28)

RX(110)    E    +    T    ==>    AL



AL  
YIELD 56%

RX(10)       RCT    E 5979-85-1  
              RGT    M 108-24-7 Ac2O  
              PRO    P 43160-23-2

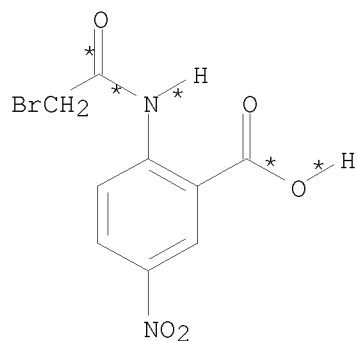
RX(22)       RCT    T 870-46-2, P 43160-23-2  
              PRO    AF 138639-40-4

RX(28)       RCT    AF 138639-40-4  
              RGT    AJ 64-19-7 AcOH  
              PRO    AL 138639-34-6

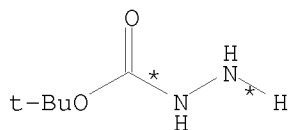
RX(112) OF 131 COMPOSED OF RX(11), RX(25), RX(31)

RX(112)    K    +    T    ==>    AO

10/ 562,112

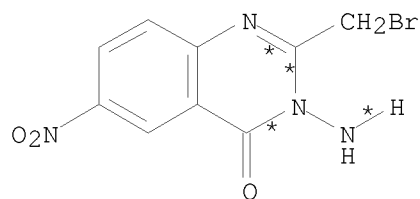


K



T

3  
STEPS  
→



AO

YIELD 76%

RX(11) RCT K 138639-68-6  
RGT M 108-24-7 Ac<sub>2</sub>O  
PRO Q 138639-62-0

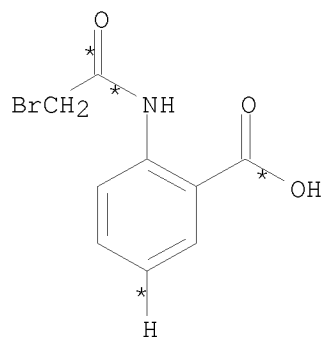
RX(25) RCT T 870-46-2, Q 138639-62-0  
PRO AH 138639-42-6

RX(31) RCT AH 138639-42-6  
RGT AJ 64-19-7 AcOH  
PRO AO 138639-47-1

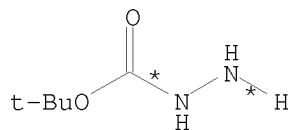
RX(113) OF 131 COMPOSED OF RX(6), RX(11), RX(25), RX(31)

RX(113) E + T ==> AO

10/ 562,112

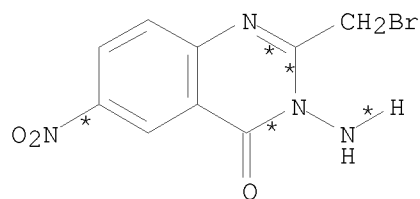


E



T

4  
STEPS  
→



AO

YIELD 76%

RX(6)      RCT    E 5979-85-1  
             RGT    J 7697-37-2 HNO3  
             PRO    K 138639-68-6

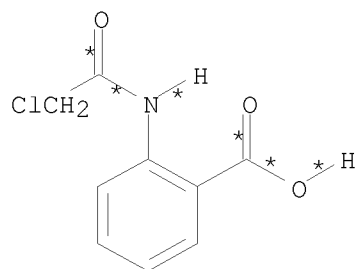
RX(11)     RCT    K 138639-68-6  
             RGT    M 108-24-7 Ac2O  
             PRO    Q 138639-62-0

RX(25)     RCT    T 870-46-2, Q 138639-62-0  
             PRO    AH 138639-42-6

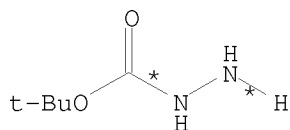
RX(31)     RCT    AH 138639-42-6  
             RGT    AJ 64-19-7 AcOH  
             PRO    AO 138639-47-1

RX(124) OF 131 COMPOSED OF RX(7), RX(18), RX(26), RX(35)  
RX(124)    C    +    T    +    AR    ==>    AS

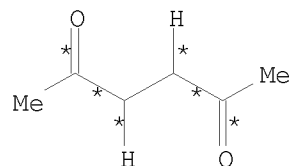
10/ 562,112



C

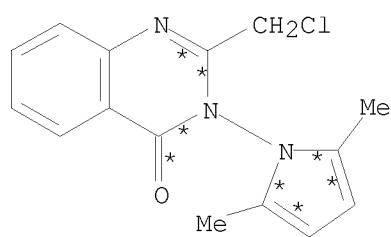


T



AR

4  
STEPS  
→



AS  
YIELD 67%

RX(7)      RCT    C 14422-49-2  
              RGT    M 108-24-7 Ac2O  
              PRO    L 98592-35-9

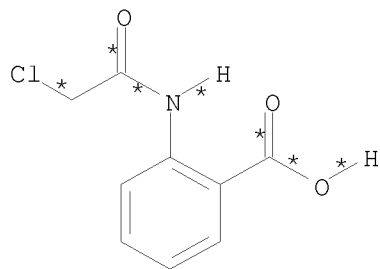
RX(18)     RCT    T 870-46-2, L 98592-35-9  
              PRO    AC 138639-39-1

RX(26)     RCT    AC 138639-39-1  
              RGT    AJ 64-19-7 AcOH  
              PRO    AI 138639-45-9

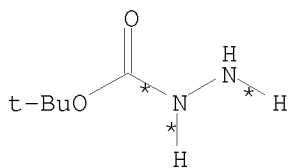
RX(35)     RCT    AR 110-13-4, AI 138639-45-9  
              PRO    AS 138639-50-6

RX(130) OF 131 COMPOSED OF RX(7), RX(18), RX(26), RX(35), RX(42)  
RX(130)    C   +   T   +   AR   ==>   BB

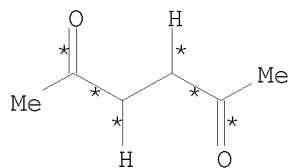
10/ 562,112



C

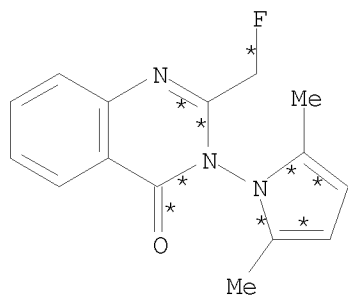


T



AR

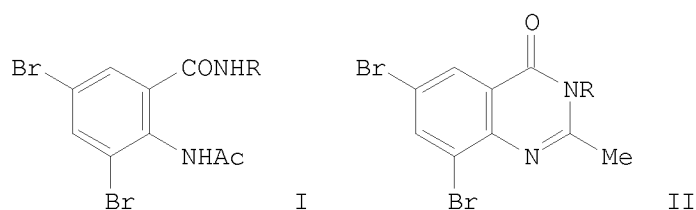
5  
STEPS  
→



BB  
YIELD 27%

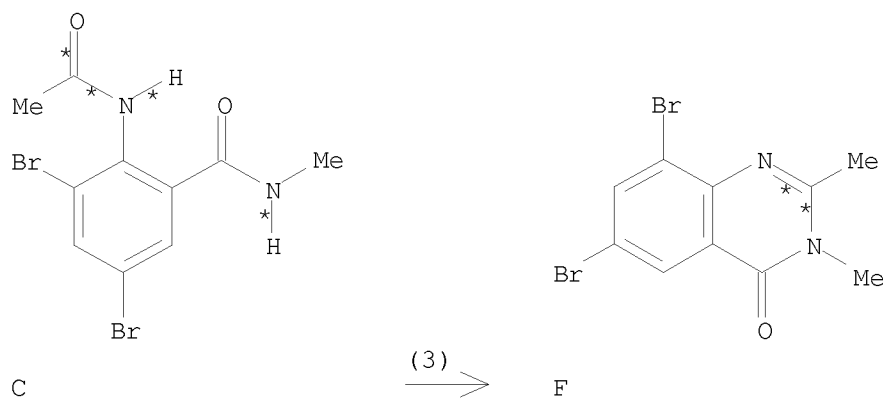
RX(7)	RCT	C 14422-49-2
	RGT	M 108-24-7 Ac2O
	PRO	L 98592-35-9
RX(18)	RCT	T 870-46-2, L 98592-35-9
	PRO	AC 138639-39-1
RX(26)	RCT	AC 138639-39-1
	RGT	AJ 64-19-7 AcOH
	PRO	AI 138639-45-9
RX(35)	RCT	AR 110-13-4, AI 138639-45-9
	PRO	AS 138639-50-6
RX(42)	RCT	AS 138639-50-6
	RGT	BC 7789-23-3 KF
	PRO	BB 138639-51-7

L3 ANSWER 143 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 116:151715 CASREACT  
 TITLE: Factors affecting cyclization of N-substituted  
 2-acylamino-3,5-dibromobenzamides to 2,3-disubstituted  
 6,8-dibromoquinazolin-4-ones  
 AUTHOR(S): Ismail, M. Fekry; Emara, Samir A.; Enayat, E. I.;  
 Mustafa, Omina E. A.  
 CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt  
 SOURCE: Polish Journal of Chemistry (1991), 65(7-8), 1259-63  
 CODEN: PJCHDQ; ISSN: 0137-5083  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



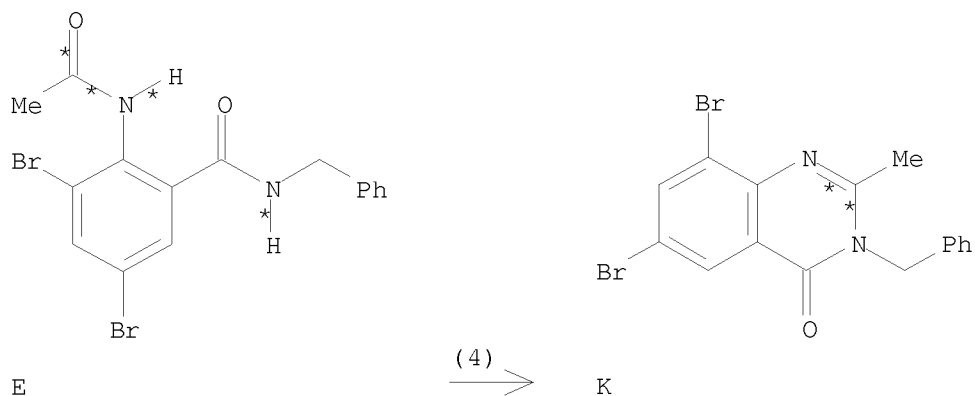
AB Cyclization of (acetylamino)dibromobenzamides I (R = Me, CH<sub>2</sub>Ph, Ph) in the presence of an amine base gave quinazolinones II. The cyclization process was dependent on basicity of the base, polarity of the medium, reaction time, and the nature of the N-substituent.

RX(3) OF 7 ...C ==> F



RX(3) RCT C 86993-54-6  
 RGT G 75-04-7 EtNH<sub>2</sub>, H 109-89-7 Et<sub>2</sub>NH, I 121-44-8 Et<sub>3</sub>N, J 1310-73-2  
 NaOH  
 PRO F 86993-61-5  
 NTE DITRI

RX(4) OF 7 ...E ==> K

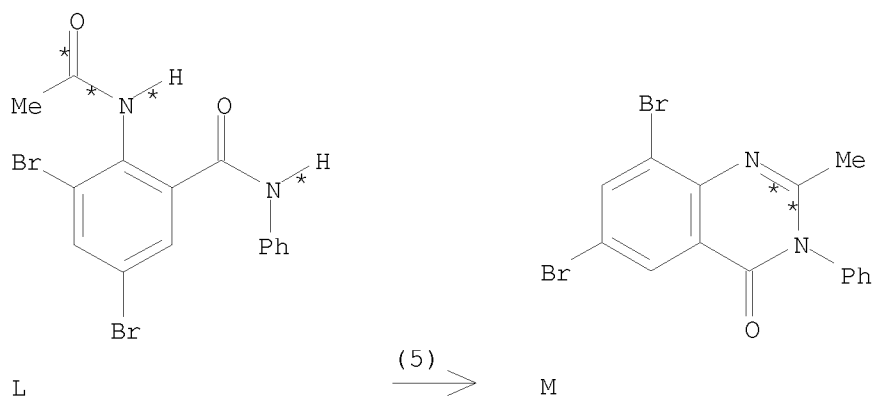


```

RX(4)      RCT  E 86993-56-8
           RGT  G 75-04-7 EtNH2, H 109-89-7 Et2NH, I 121-44-8 Et3N, J 1310-73-2
           NaOH
           PRO  K 86993-63-7
           NTE  DITRI

```

RX(5) OF 7 L ==&gt; M



```

RX(5)      RCT  L 78993-24-5
           RGT  G 75-04-7 EtNH2, H 109-89-7 Et2NH, I 121-44-8 Et3N, J 1310-73-2
           NaOH
           PRO  M 4145-21-5
           NTE  DITRI

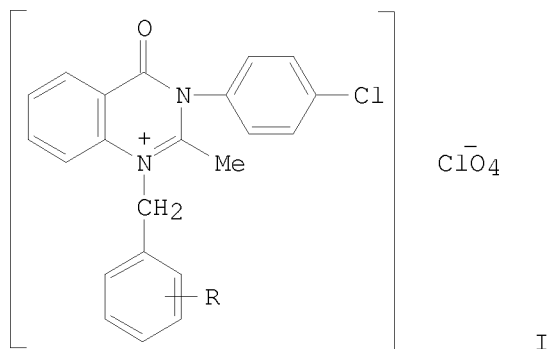
```

L3 ANSWER 144 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 116:143879 CASREACT  
 TITLE: Benzyl phenyl quirazolinone perchlorates displaying  
 analgesic, anticonvulsive, and antimicrobial activity  
 INVENTOR(S): Chernobrovin, N. I.; Kozhevnikov, Yu. V.; Morozova, G.  
 E.; Zalesov, V. S.; Plaksina, A. N.

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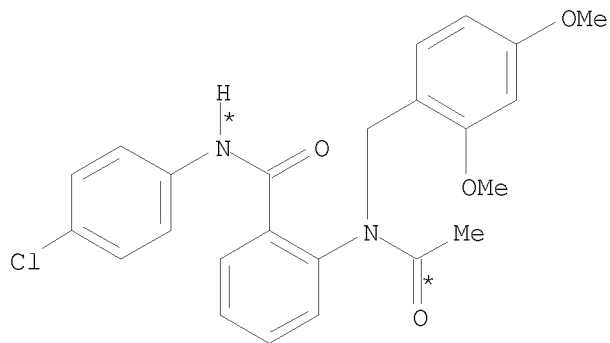
PATENT ASSIGNEE(S): Perm Pharmaceutical Institute, USSR  
SOURCE: U.S.S.R. From: Otkrytiya, Izobret. 1991, (28), 258.  
CODEN: URXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Russian  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 1110140	A1	19910730	SU 1983-3554870	19830217
PRIORITY APPLN. INFO.: GI			SU 1983-3554870	19830217

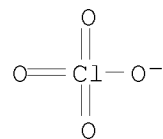


AB The title compds. [I: R = (OCH<sub>3</sub>)<sub>2</sub>] display analgesic, anticonvulsive, and antimicrobial activity.

RX(6) OF 14 L ==> M



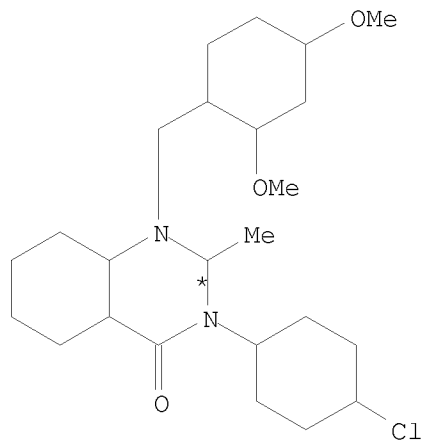
L



M: CM 1  
YIELD 90%



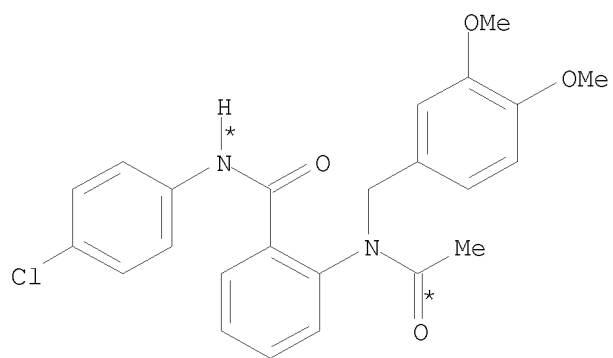
10/ 562,112



M: CM 2  
YIELD 90%

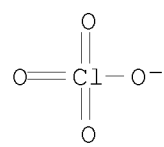
RX(6)      RCT    L 143424-27-5  
             RGT    N 7601-90-3 HClO4  
             PRO    M 139755-24-1

RX(7) OF 14      ...K ==> O



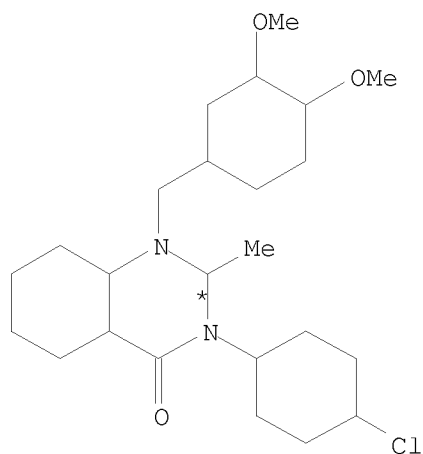
K

(7) →



O: CM 1  
YIELD 84%

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O: CM 2  
YIELD 84%

RX(7) RCT K 143424-31-1  
RGT N 7601-90-3 HClO4  
PRO O 143579-10-6

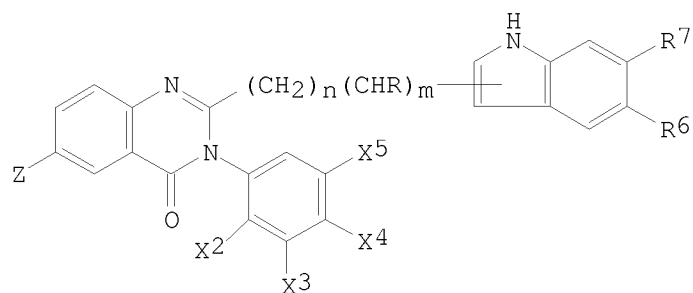
L3 ANSWER 145 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 116:128964 CASREACT  
TITLE: Preparation of 2-indolyl-3-phenyl-4-quinazolinones as  
cholecystokinin antagonists  
INVENTOR(S): Yu, Melvin J.; Mccowan, Jefferson R.; Thrasher, K.  
Jeff  
PATENT ASSIGNEE(S): Eli Lilly and Co., USA  
SOURCE: U.S., 10 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5075313	A	19911224	US 1990-581943	19900913
CA 2050994	A1	19920314	CA 1991-2050994	19910909
ZA 9107149	A	19920527	ZA 1991-7149	19910909
JP 04247080	A	19920903	JP 1991-227902	19910909
FI 9104262	A	19920314	FI 1991-4262	19910910
HU 59128	A2	19920428	HU 1991-2921	19910910
NO 9103579	A	19920316	NO 1991-3579	19910911
AU 9183829	A	19920319	AU 1991-83829	19910911
AU 641043	B2	19930909		
CZ 279774	B6	19950614	CZ 1991-2799	19910911
EP 475755	A1	19920318	EP 1991-308324	19910912
EP 475755	B1	19950927		

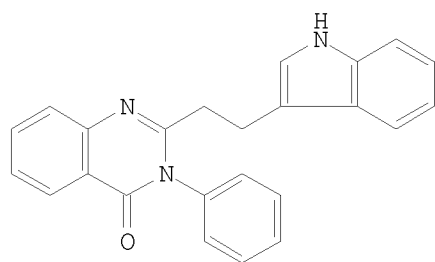
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE

10/ 562,112

CN 1059722	A	19920325	CN 1991-108887	19910912
ES 2078455	T3	19951216	ES 1991-308324	19910912
US 5196427	A	19930323	US 1991-763104	19910920
PRIORITY APPLN. INFO.:			US 1990-581943	19900913
OTHER SOURCE(S):			MARPAT 116:128964	
GI				



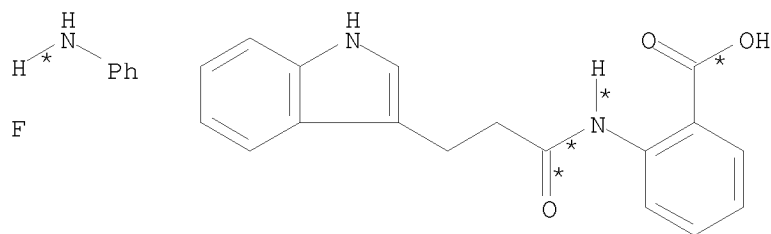
I



II

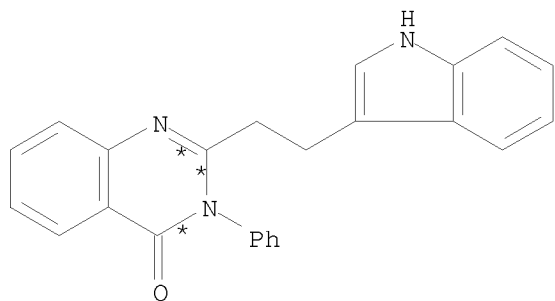
AB Title compds. (I;  $n = 1, 2$ ;  $m = 0, 1$ ;  $R = H, \text{ alkyl}, \text{ PhCH}_2, \text{ Ph}$ ;  $Z = H, \text{ halo}$ ;  $X_2-X_5 = H, \text{ halo}, \text{ CF}_3, \text{ alkoxy}, \text{ alkyl}, \text{ alkylthio}, \text{ amino}$ ;  $R_6, R_7 = H, \text{ alkyl}, \text{ alkoxy}, \text{ halo}, \text{ CF}_3$ ), were prepared Thus, 3-(3-indolyl)propionic acid and Me anthranilate in THF were refluxed with carbonyldiimidazole and pyridinium p-toluenesulfonate to give 70% 3-(3-indolyl)-N-(2-methoxycarbonylphenyl)propionamide. This was saponified with NaOH/MeOH followed by treatment with aniline, carbonyldiimidazole, and pyridinium p-toluenesulfonate in refluxing THF to give title compound II. I bound to CCK receptors in mouse brain membrane preps. with IC<sub>50</sub>'s of 0.019-1.2  $\mu\text{M}$ . I are useful in treating gastrointestinal, CNS, and appetite disorders.

RX(3) OF 6 ...F + E ==> G



(3) >

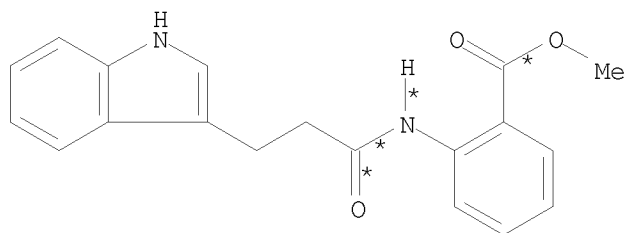
10/ 562,112



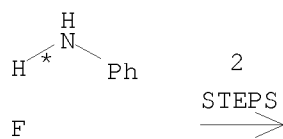
G

RX(3) RCT F 62-53-3, E 139543-67-2  
 PRO G 133040-57-0  
 CAT 530-62-1 Diimidazolyl ketone

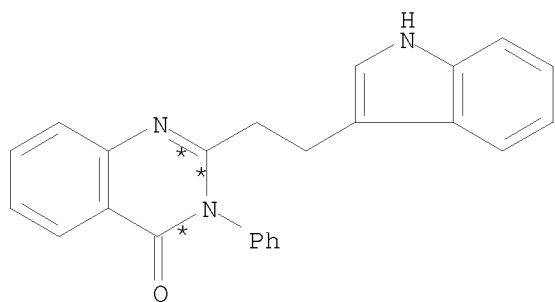
RX(5) OF 6 COMPOSED OF RX(2), RX(3)  
 RX(5) C + F ==> G



C



F



G

RX(2) RCT C 139543-66-1  
 PRO E 139543-67-2

RX(3) RCT F 62-53-3, E 139543-67-2

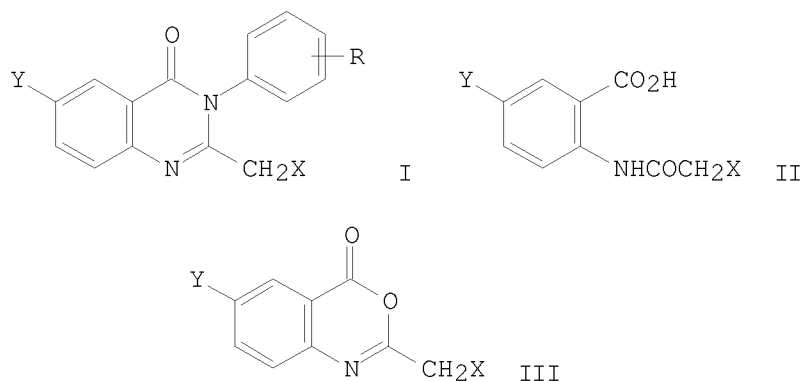
PRO G 133040-57-0  
 CAT 530-62-1 Diimidazolyl ketone

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 146 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 115:114535 CASREACT  
 TITLE: Preparation of quinazolinone derivatives as intermediates for minor tranquilizers and neuroleptics  
 INVENTOR(S): Myashita, Masahiko  
 PATENT ASSIGNEE(S): Nippon Synthetic Chemical Industry Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03058977	A	19910314	JP 1989-196366	19890727
PRIORITY APPLN. INFO.:			JP 1989-196366	19890727
OTHER SOURCE(S):			MARPAT 115:114535	

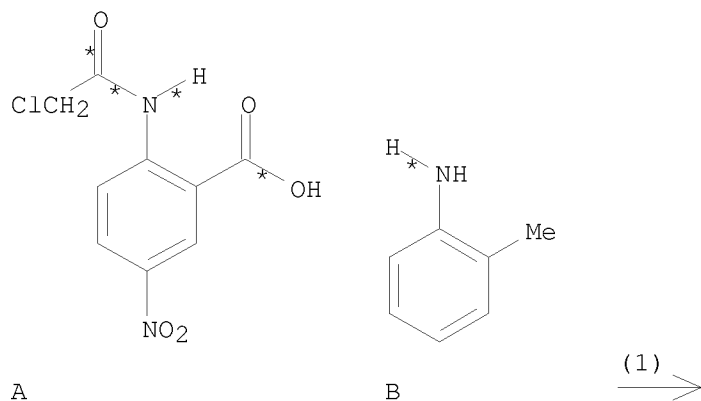
GI



AB The title derivs. I (R = alkyl; X = halo; Y = alkyl, halo, alkylamino, NO<sub>2</sub>), useful as intermediates for I (X = F; Y = NH<sub>2</sub>) which are minor tranquilizers and neuroleptics, are prepared by cyclization of N-acylantranilic acids II (X, Y = same as I) with Ac<sub>2</sub>O at a mol ratio of 1:(0.9-1.2) and treatment of the resulting benzoxazinones III (X, Y = same as I) with RC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> without further purification Thus, a solution of 0.023 mol II (X = Cl, Y = NO<sub>2</sub>) in toluene was refluxed with 0.025 mol Ac<sub>2</sub>O for 6 h and further refluxed with o-MeC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> for 3 h to give 87% I (R = 2-Me, X = Cl, Y = NO<sub>2</sub>).

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RX(1) OF 1      A + B ==> C



C  
YIELD 87%

RX(1)      RCT    A 135590-27-1

STAGE(1)

RGT    D 108-24-7 Ac2O

SOL    108-88-3 PhMe

STAGE(2)

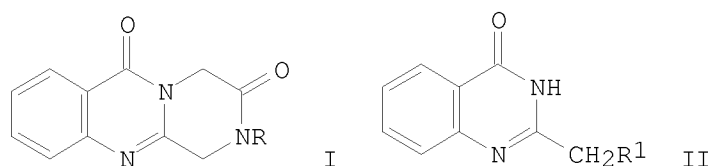
RCT    B 95-53-4

PRO    C 61899-76-1

L3    ANSWER 147 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER:    115:29242    CASREACT  
TITLE:    A new synthesis of  
2-aryl-2H-pyrazino[2,1-b]quinazoline-3,6(1H,4H)-diones  
AUTHOR(S):    Reddy, P. S. N.; Nagaraju, C.  
CORPORATE SOURCE:    Dep. Chem., Osmania Univ., Hyderabad, 500 007, India  
SOURCE:    Synthetic Communications (1991), 21(2), 173-81  
CODEN: SYNCAV; ISSN: 0039-7911  
DOCUMENT TYPE:    Journal  
LANGUAGE:    English

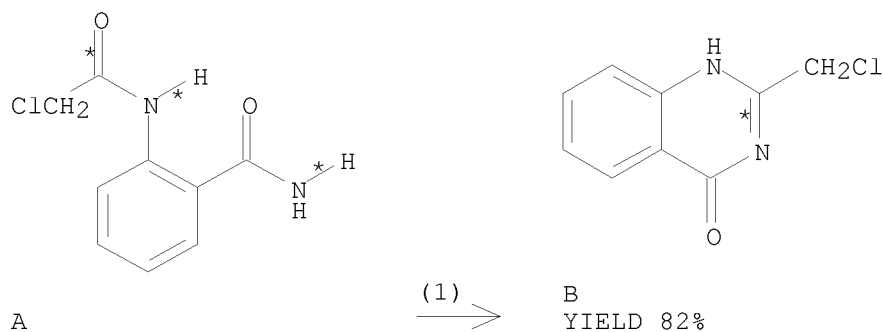
10/ 562,112

GI



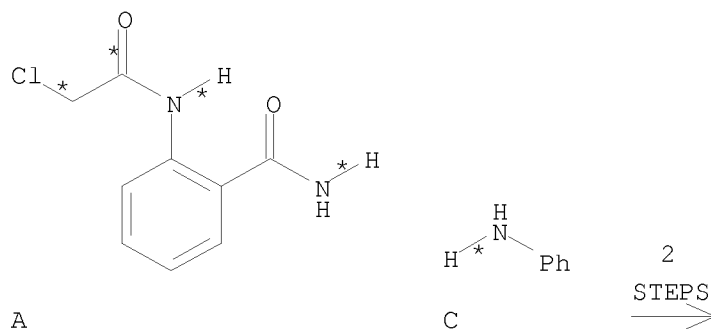
AB Six title compds. I ( R = Ph, substituted Ph) were prepared starting from (2-chloromethyl)quinazolinone II (R1 = Cl) in 3 steps involving condensation with RNH2 to give II (R1 = NHR), condensation with chloroacetic anhydride or ClCH2COCl to give II (R1 = NRCOCH2Cl) and dehydrochlorination-cyclization with Et3N in dioxane at room temperature

RX(1) OF 19      A ==> B...

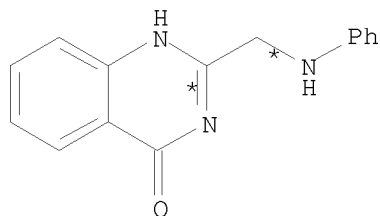


RX(1)      RCT    A 21721-78-8  
             PRO    B 3817-05-8  
             NTE    Polyphosphate Et ester solvent

RX(8) OF 19 COMPOSED OF RX(1), RX(2)  
RX(8)      A + C ==> D



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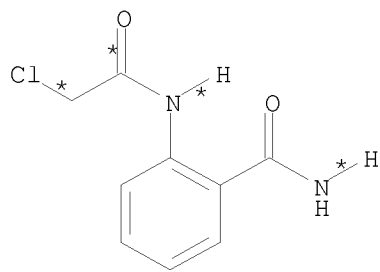
D  
YIELD 52%

RX(1) RCT A 21721-78-8  
PRO B 3817-05-8  
NTE Polyphosphate Et ester solvent

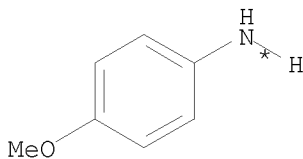
RX(2) RCT B 3817-05-8, C 62-53-3  
PRO D 3817-06-9  
SOL 64-17-5 EtOH

RX(9) OF 19 COMPOSED OF RX(1), RX(4)

RX(9) A + I ==> J

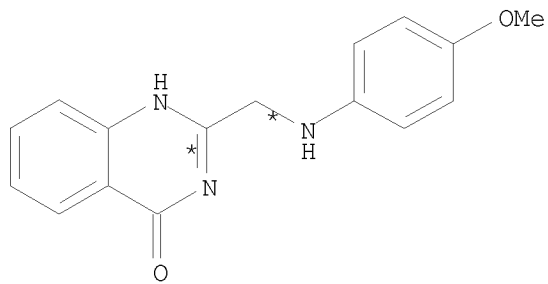


A



I

2  
STEPS  
→



J  
YIELD 42%

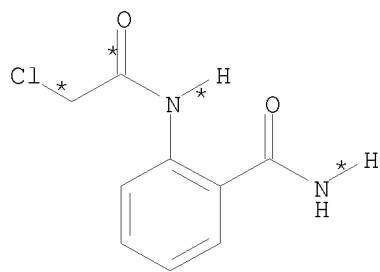


10/ 562,112

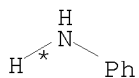
RX(1) RCT A 21721-78-8  
PRO B 3817-05-8  
NTE Polyphosphate Et ester solvent

RX(4) RCT B 3817-05-8, I 104-94-9  
PRO J 134577-52-9  
SOL 64-17-5 EtOH

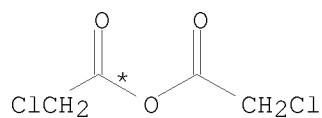
RX(14) OF 19 COMPOSED OF RX(1), RX(2), RX(3)  
RX(14) A + C + F ==> G



A

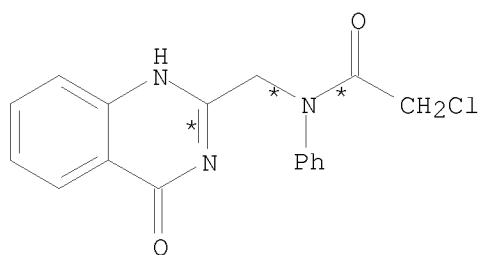


C



F

3  
STEPS  
→



G  
YIELD 72%

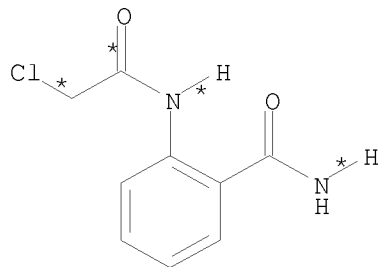
RX(1) RCT A 21721-78-8  
PRO B 3817-05-8  
NTE Polyphosphate Et ester solvent

RX(2) RCT B 3817-05-8, C 62-53-3  
PRO D 3817-06-9  
SOL 64-17-5 EtOH

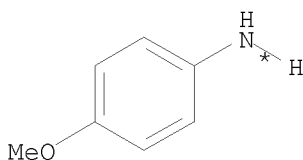
RX(3) RCT D 3817-06-9, F 541-88-8  
PRO G 134577-55-2  
SOL 75-09-2 CH2Cl2

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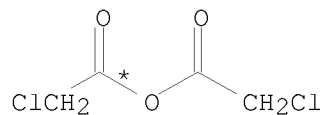
RX(15) OF 19 COMPOSED OF RX(1), RX(4), RX(6)  
RX(15) A + I + F ==> N



A

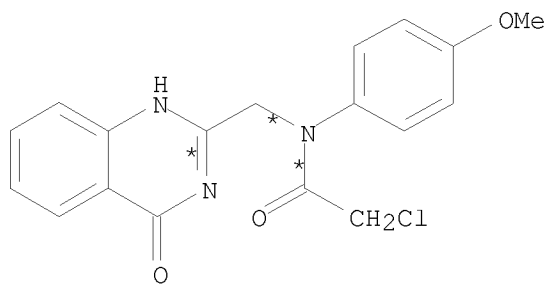


I



F

3  
STEPS  
→



N  
YIELD 84%

RX(1) RCT A 21721-78-8  
PRO B 3817-05-8  
NTE Polyphosphate Et ester solvent

RX(4) RCT B 3817-05-8, I 104-94-9  
PRO J 134577-52-9  
SOL 64-17-5 EtOH

RX(6) RCT J 134577-52-9, F 541-88-8  
PRO N 134577-58-5  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

TITLE: Synthesis and reactions of  
2-( $\alpha$ -benzoylamino-p-chlorostyryl)-3,1(4H)-  
benzoxazin-4-one with some nucleophilic reagents:  
synthesis of quinazolinone, tetrazole and  
benzimidazole derivatives

AUTHOR(S): El-Khamry, Abdel Momen A.; El-Nagdy, S.; Shaban, M. E.

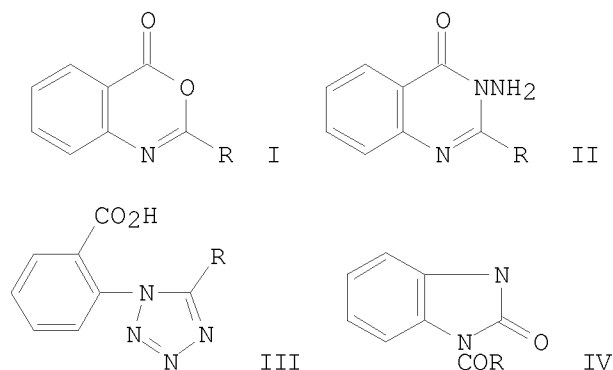
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt

SOURCE: Egyptian Journal of Chemistry (1990), Volume Date  
1988, 31(2), 261-9  
CODEN: EGJCA3; ISSN: 0367-0422

DOCUMENT TYPE: Journal

LANGUAGE: English

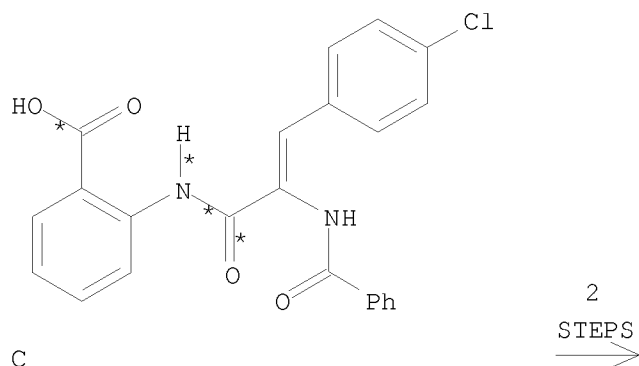
GI



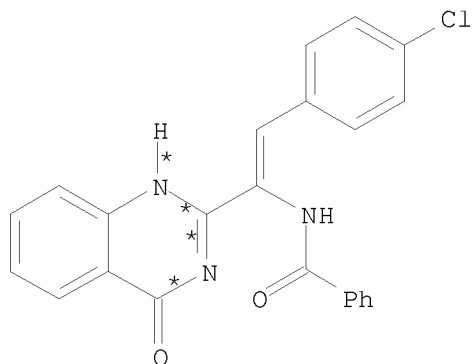
AB Treating benzoxazinone I (R = p-ClC<sub>6</sub>H<sub>4</sub>CH:CNHBz throughout) with R<sub>1</sub>NH<sub>2</sub> (R<sub>1</sub> = Et, PhCH<sub>2</sub>, 4-pyridyl, p-tolyl, p-MeOC<sub>6</sub>H<sub>4</sub>, NH<sub>2</sub>, PhNH) gave 60-85% o-R<sub>1</sub>NHCOC<sub>6</sub>H<sub>4</sub>NHCOR. Treating I with N<sub>2</sub>H<sub>4</sub> in BuOH gave 65% quinazoline II which condensed with R<sub>2</sub>CHO (R<sub>2</sub> = p-ClC<sub>6</sub>H<sub>4</sub>, p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, p-Me<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>) gave 60-70% of the corresponding Schiff bases. Addnl. obtained was tetrazole III and benzimidazolone IV.

RX(34) OF 71 COMPOSED OF RX(3), RX(13)

RX(34) C ==> Y



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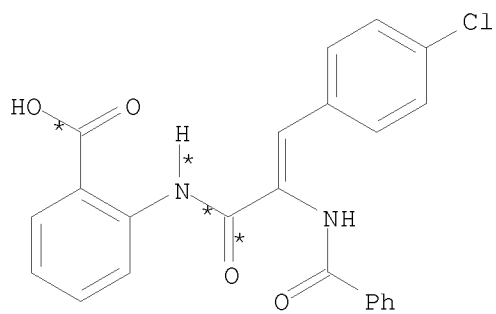


Y

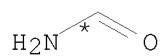
RX(3)      RCT    C 132994-47-9  
              PRO    D 132994-48-0  
              CAT    108-24-7 Ac2O

RX(13)     RCT    D 132994-48-0  
              PRO    Y 132994-58-2  
              CAT    631-61-8 NH4OAc

RX(35) OF 71 COMPOSED OF RX(3), RX(14)  
 RX(35)      C    +    AA    ==>    Y



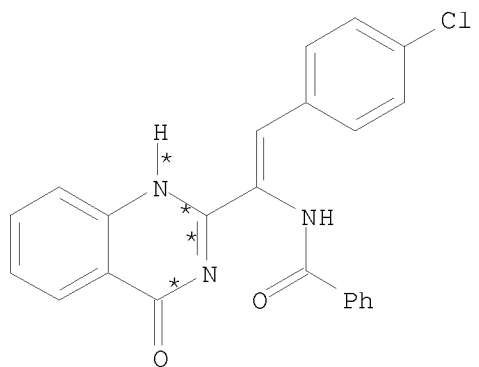
C



AA

2  
 STEPS  
 →

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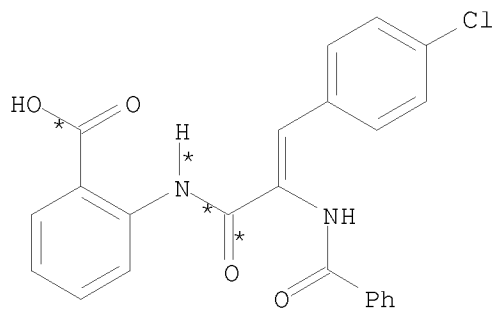


Y

RX(3)        RCT    C 132994-47-9  
              PRO    D 132994-48-0  
              CAT    108-24-7 Ac2O

RX(14)       RCT    D 132994-48-0, AA 75-12-7  
              PRO    Y 132994-58-2

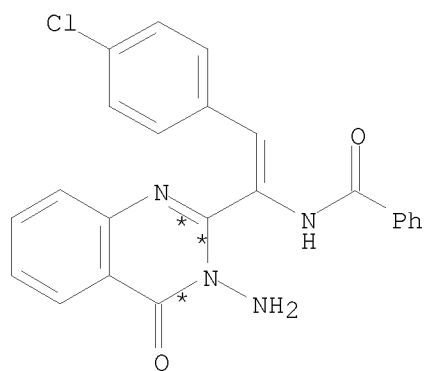
RX(36) OF 71 COMPOSED OF RX(3), RX(15)  
RX(36)       C    ==>    AB



C

2  
STEPS  
→

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AB

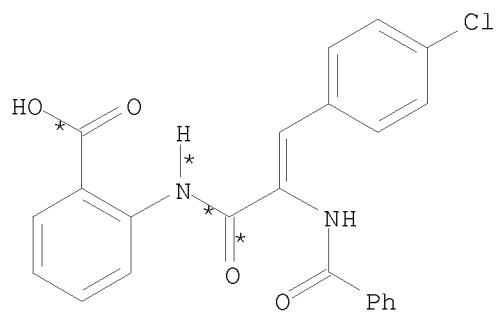
YIELD 65%

RX(3)      RCT    C 132994-47-9  
             PRO    D 132994-48-0  
             CAT    108-24-7 Ac2O

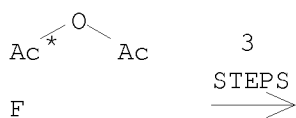
RX(15)      RCT    D 132994-48-0  
             RGT    R 302-01-2 N2H4  
             PRO    AB 132994-59-3

RX(59) OF 71 COMPOSED OF RX(3), RX(15), RX(16)

RX(59)      C    +    F    ==>    AC

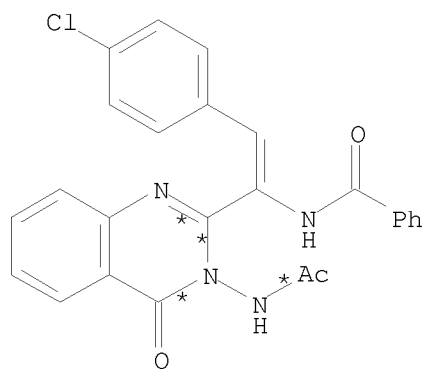


C



F

10/ 562,112



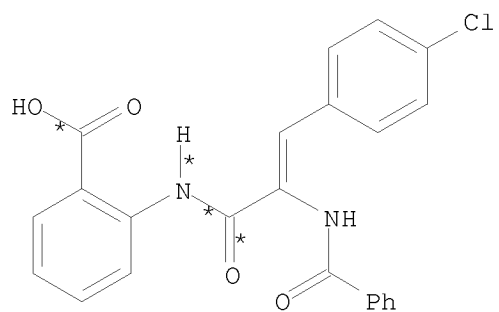
AC

RX(3)      RCT    C 132994-47-9  
              PRO    D 132994-48-0  
              CAT    108-24-7 Ac2O

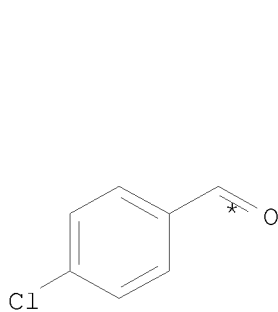
RX(15)     RCT    D 132994-48-0  
              RGT    R 302-01-2 N2H4  
              PRO    AB 132994-59-3

RX(16)     RCT    AB 132994-59-3, F 108-24-7  
              PRO    AC 132994-60-6

RX(60) OF 71 COMPOSED OF RX(3), RX(15), RX(17)  
 RX(60)      C    +    AD    ==>    AE



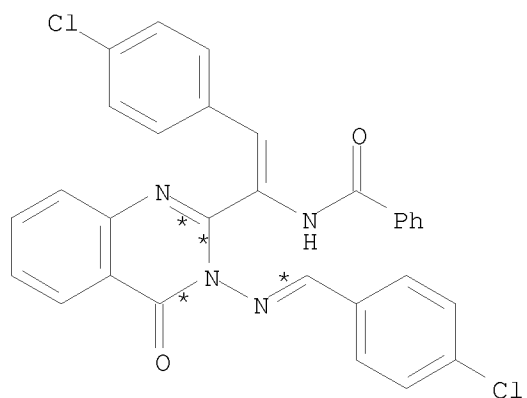
C



AD

3  
 STEPS  
 →

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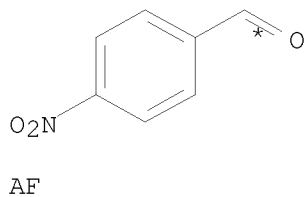
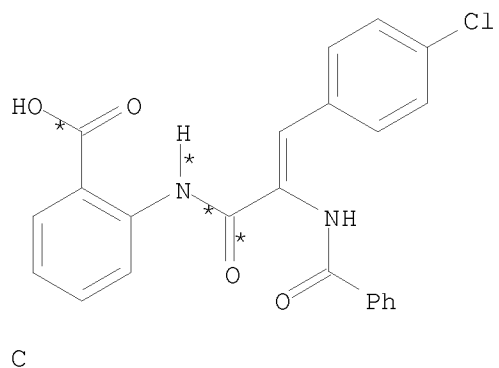
AE  
YIELD 65%

RX(3) RCT C 132994-47-9  
PRO D 132994-48-0  
CAT 108-24-7 Ac2O

RX(15) RCT D 132994-48-0  
RGT R 302-01-2 N2H4  
PRO AB 132994-59-3

RX(17) RCT AB 132994-59-3, AD 104-88-1  
PRO AE 132994-61-7

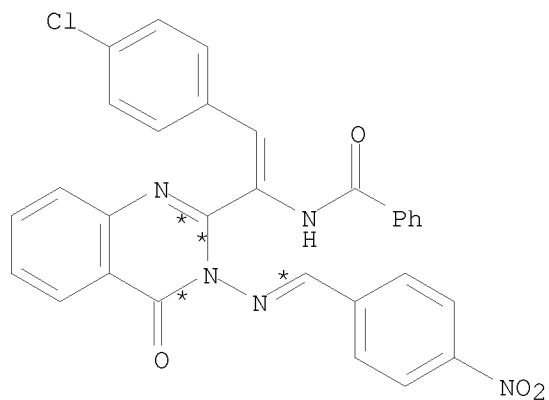
RX(61) OF 71 COMPOSED OF RX(3), RX(15), RX(18)  
RX(61) C + AF ==> AG



3  
STEPS  
→



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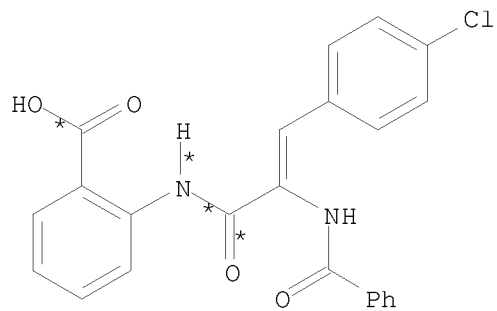
AG  
YIELD 60%

RX(3) RCT C 132994-47-9  
PRO D 132994-48-0  
CAT 108-24-7 Ac2O

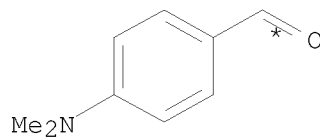
RX(15) RCT D 132994-48-0  
RGT R 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO AB 132994-59-3

RX(18) RCT AB 132994-59-3, AF 555-16-8  
PRO AG 132994-62-8

RX(62) OF 71 COMPOSED OF RX(3), RX(15), RX(19)  
RX(62) C + AH ==> AI



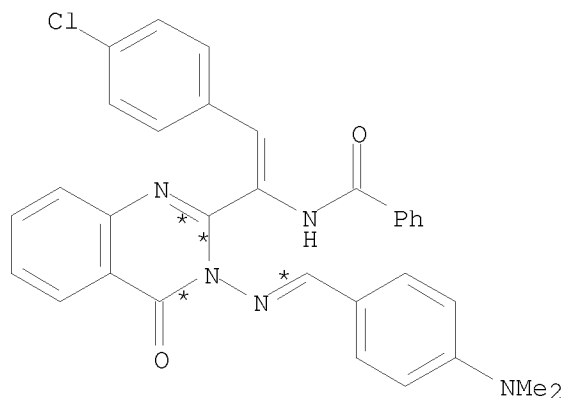
C



AH

3  
STEPS  
→

10/ 562,112



AI  
YIELD 70%

RX(3) RCT C 132994-47-9  
PRO D 132994-48-0  
CAT 108-24-7 Ac2O

RX(15) RCT D 132994-48-0  
RGT R 302-01-2 N2H4  
PRO AB 132994-59-3

RX(19) RCT AB 132994-59-3, AH 100-10-7  
PRO AI 133023-95-7

L3 ANSWER 149 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 114:163892 CASREACT

TITLE: Synthesis of 2-alkyl-3-aminoquinazolin-4(3H)-ones and  
their use for enantioselective aminoaziridinations  
using a chiral oxidant

AUTHOR(S): Zhalnina, G. V.; Kuznetsov, M. A.; Semenovskii, V. V.;  
Shustov, G. V.

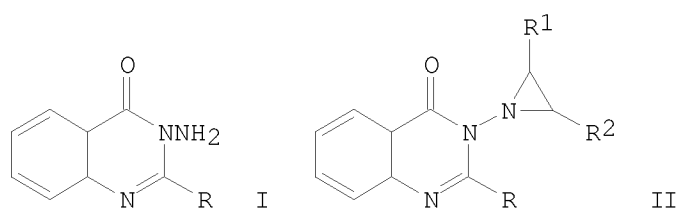
CORPORATE SOURCE: USSR

SOURCE: Vestnik Leningradskogo Universiteta, Seriya 4:  
Fizika, Khimiya (1990), (3), 72-6  
CODEN: VLUFBI; ISSN: 0024-0826

DOCUMENT TYPE: Journal

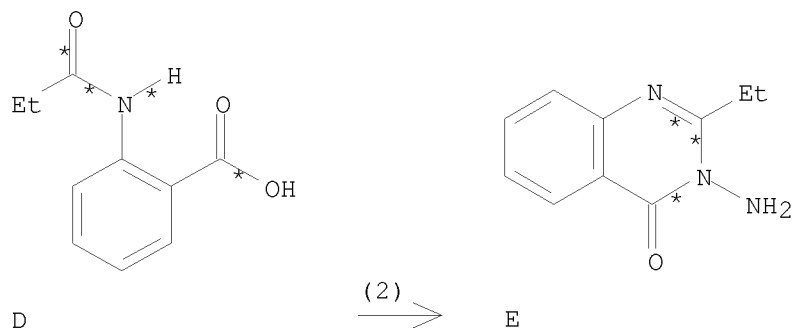
LANGUAGE: Russian

GI



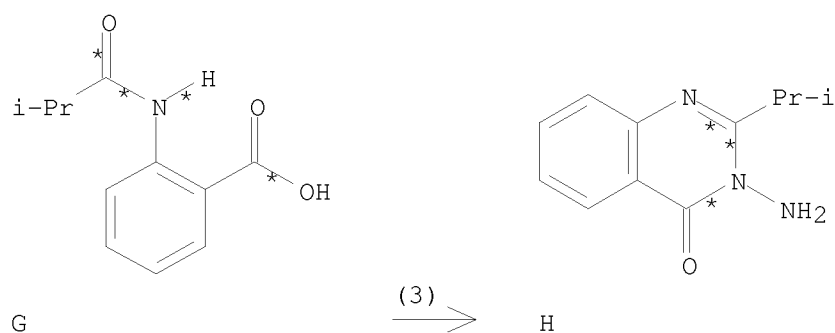
AB Aminoquinazolinone derivs. (I: R = Et, CHMe<sub>2</sub>, CMe<sub>3</sub>) were prepared from anthranilic acid Me ester. Oxidation of (I; R = Et, CHMe<sub>2</sub>) by Pb(OAc)<sub>4</sub> in the presence of excess styrene, trans-stilbene or dimethyl fumarate affords the corresponding racemic dihydroquinazolinylaziridines (II; R<sub>1</sub> = Ph, CO<sub>2</sub>Me; R<sub>2</sub> = H, Ph, CO<sub>2</sub>Me) in 50-70% yield. With optically active oxidant lead tetra-(S)-2-methylbutanoate, asym. induction is observed only for trans-stilbene.

RX(2) OF 11 ...D ==> E



RX(2)        RCT    D 19165-26-5  
               RGT    F 302-01-2 N<sub>2</sub>H<sub>4</sub>  
               PRO    E 50547-51-8

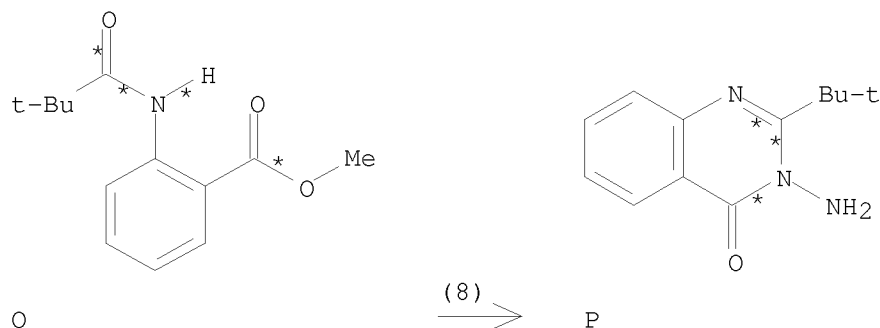
RX(3) OF 11 ...G ==> H



RX(3)        RCT    G 17840-96-9  
               RGT    F 302-01-2 N<sub>2</sub>H<sub>4</sub>  
               PRO    H 70589-51-4

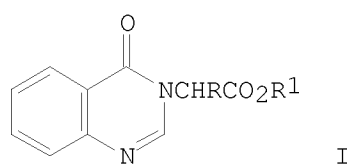
RX(8) OF 11 ...O ==> P

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RX(8)      RCT   O 84540-62-5  
              RGT   F 302-01-2 N2H4  
              PRO   P 132871-77-3

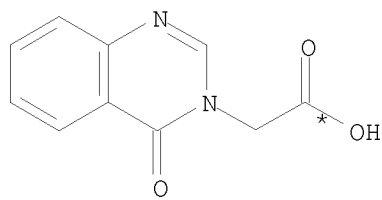
L3    ANSWER 150 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER:        114:81745    CASREACT  
 TITLE:                      Esters of quinazolin-4[3H]-on-3-ylacetic and  
                                  2-(quinazolin-4[3H]-on-3-yl)propionic acids  
 AUTHOR(S):                Fisnerova, L.; Brunova, B.; Maturova, E.; Grimova, J.  
 CORPORATE SOURCE:        Vyzk. Ustav Farm. Biochem., Prague, Czech.  
 SOURCE:                    Cesko-Slovenska Farmacie (1990), 39(6), 275-7  
                                  CODEN: CKFRAY; ISSN: 0009-0530  
 DOCUMENT TYPE:            Journal  
 LANGUAGE:                 Czech  
 GI



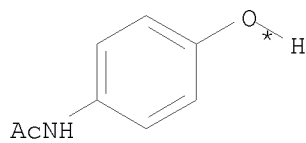
AB    Several new esters of quinazolinonylacetic I (R = H; R<sub>1</sub> = 2-benzimidazolylhydroxymethyl, 4-AcNHC<sub>6</sub>H<sub>4</sub>, substituted biphenylol) and quinazolinonylpropionic I (R = Me, R<sub>1</sub> = 2-benzimidazolylhydroxymethyl, 4-AcNHC<sub>6</sub>H<sub>4</sub>) acid were prepared. The analgetic efficacy of these compds. was comparable to that of aminophenazone, while their acute toxicity in mice was significantly lower.

RX(2) OF 8      D + E ==> F

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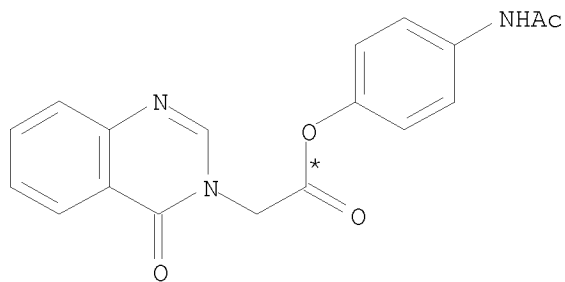


D



E

(2)  $\longrightarrow$

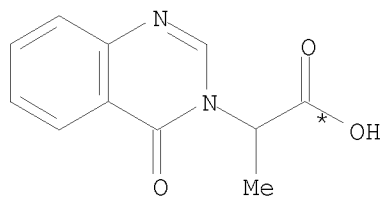


F

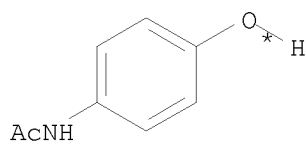
YIELD 60%

RX(2)      RCT    D 14663-53-7, E 103-90-2  
             PRO    F 131842-95-0

RX(7) OF 8      M + E ==> N



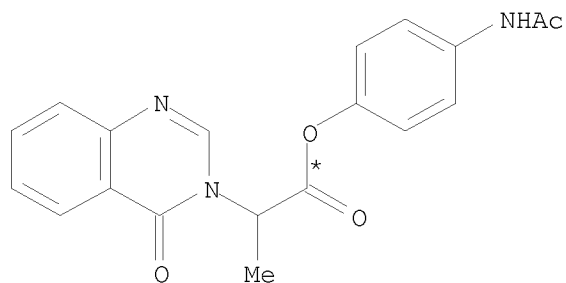
M



E

(7)  $\longrightarrow$

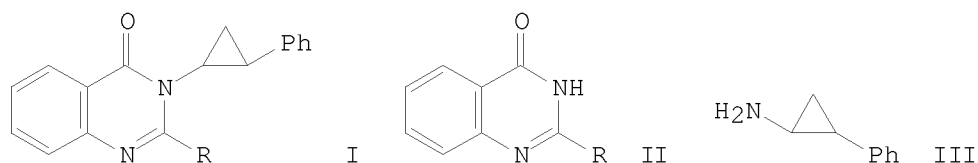
10/ 562,112



N  
YIELD 48%

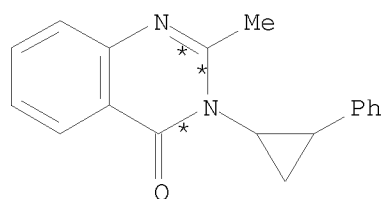
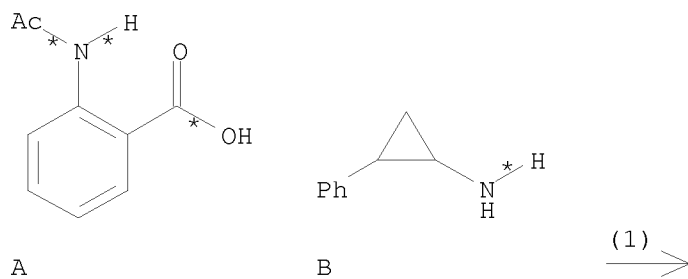
RX(7) RCT M 61381-36-0, E 103-90-2  
PRO N 131843-00-0

L3 ANSWER 151 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 114:62036 CASREACT  
TITLE: Some 4-(3H)-quinazolinones as anticonvulsants and  
monoamine oxidase inhibitors  
AUTHOR(S): Aboul-Enein, M. Nabil; Eid, A. I.; El-Azzouny, Aida A.  
CORPORATE SOURCE: Lab. Pharm. Sci., Natl. Res. Cent., Cairo, Egypt  
SOURCE: Egyptian Journal of Chemistry (1989), Volume Date  
1987, 30(6), 515-16  
CODEN: EGJCA3; ISSN: 0367-0422  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Phenylcyclopropylquinazolinones I (R = Me, Ph) were prepared by the reaction of quinazolinones II with phenylcyclopropylamine III. Various derivs., e.g., I (R = CH:CHR1 = Ph, substituted Ph) of I (R = Me) were prepared by condensation with aldehydes.

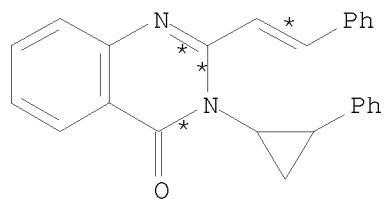
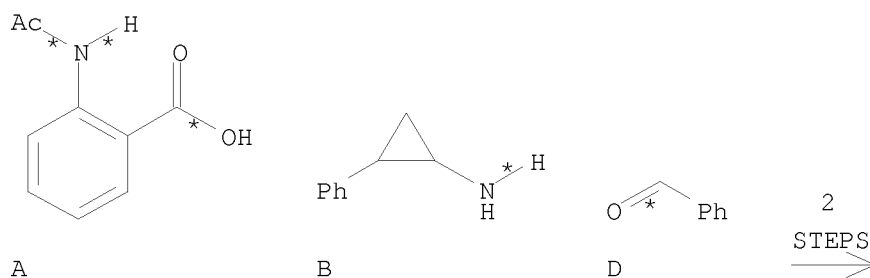
RX(1) OF 12 A + B ==> C...



C  
YIELD 50%

RX(1)            RCT    A 89-52-1, B 54-97-7  
                  PRO    C 131557-26-1

RX(8) OF 12 COMPOSED OF RX(1), RX(2)  
RX(8)            A + B + D  $\implies$  E



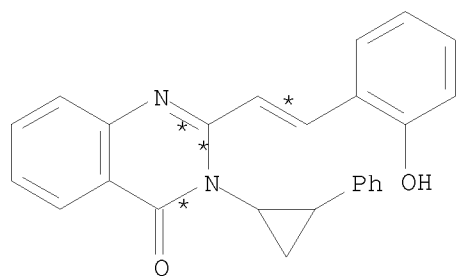
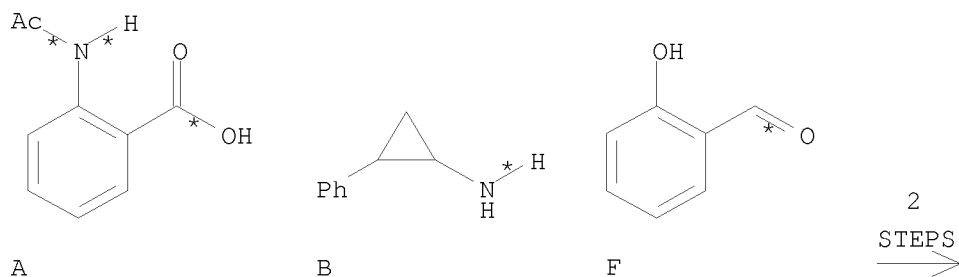
E  
YIELD 82%

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RX(1) RCT A 89-52-1, B 54-97-7  
PRO C 131557-26-1

RX(2) RCT C 131557-26-1, D 100-52-7  
PRO E 131557-28-3

RX(9) OF 12 COMPOSED OF RX(1), RX(3)  
RX(9) A + B + F ==> G



G  
YIELD 75%

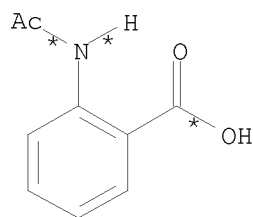
RX(1) RCT A 89-52-1, B 54-97-7  
PRO C 131557-26-1

RX(3) RCT C 131557-26-1, F 90-02-8  
PRO G 131557-29-4

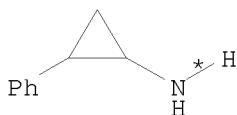
RX(10) OF 12 COMPOSED OF RX(1), RX(4)  
RX(10) A + B + H ==> I



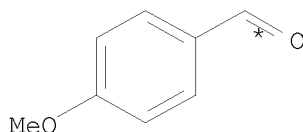
10/ 562,112



A

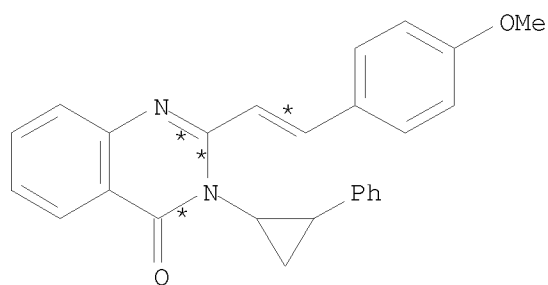


B



H

2  
STEPS  
→

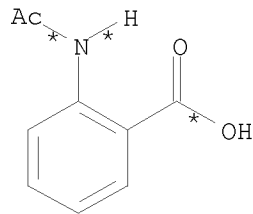


I  
YIELD 78%

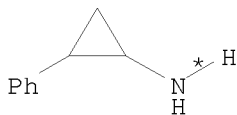
RX(1) RCT A 89-52-1, B 54-97-7  
PRO C 131557-26-1

RX(4) RCT C 131557-26-1, H 123-11-5  
PRO I 131557-30-7

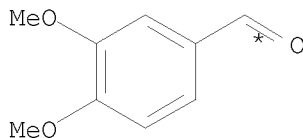
RX(11) OF 12 COMPOSED OF RX(1), RX(5)  
RX(11) A + B + J ==> K



A



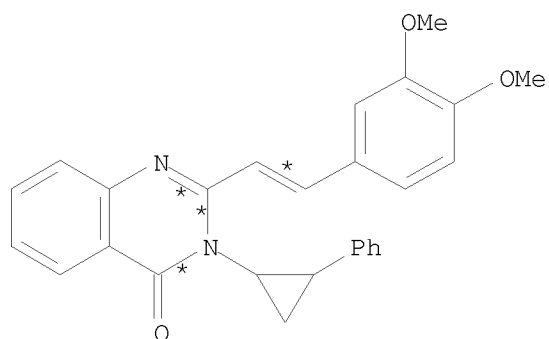
B



J

2  
STEPS  
→

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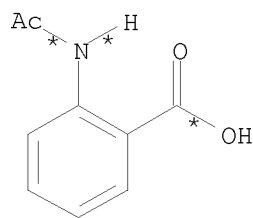


K

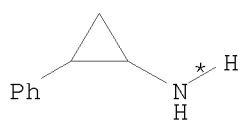
RX(1) RCT A 89-52-1, B 54-97-7  
PRO C 131557-26-1

RX(5) RCT C 131557-26-1, J 120-14-9  
PRO K 131557-31-8  
CAT 110-86-1 Pyridine

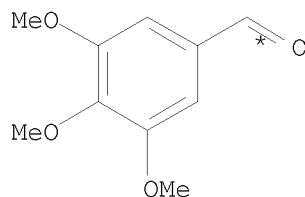
RX(12) OF 12 COMPOSED OF RX(1), RX(6)  
RX(12) A + B + M ==> N



A

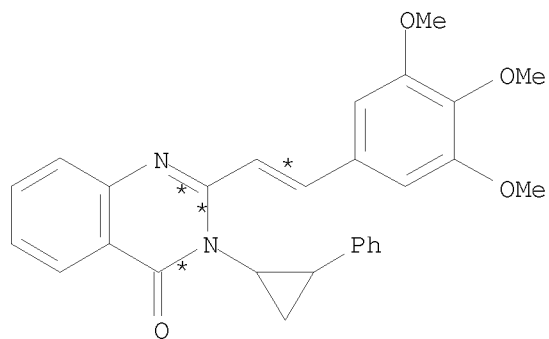


B



M

2  
STEPS  
→



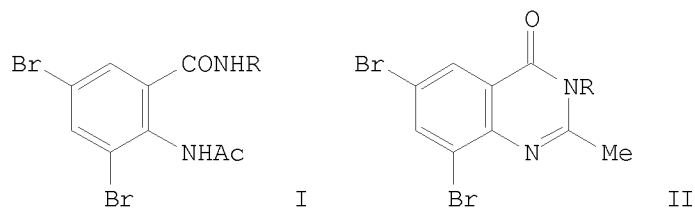
N

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RX(1) RCT A 89-52-1, B 54-97-7  
PRO C 131557-26-1

RX(6) RCT C 131557-26-1, M 86-81-7  
PRO N 131557-32-9  
CAT 110-86-1 Pyridine

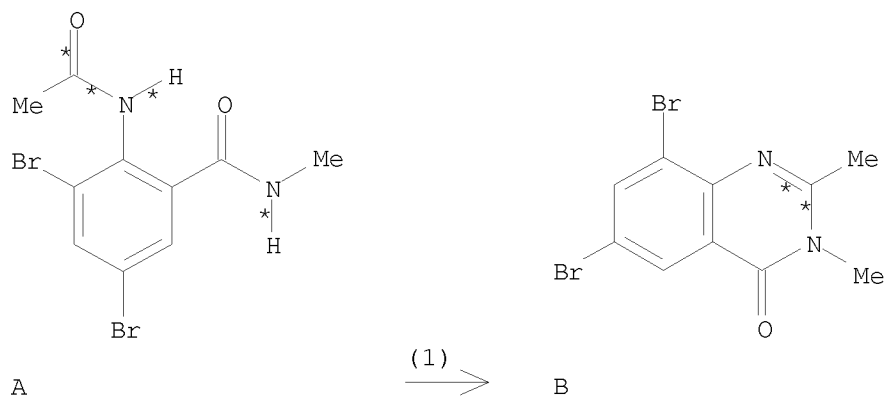
L3 ANSWER 152 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 114:23917 CASREACT  
TITLE: Factors affecting cyclization of N-substituted  
2-(acetylamino)-3,5-dibromobenzamide to  
2,3-disubstituted 6,8-dibromoquinazolin-4-ones  
AUTHOR(S): Ismail, M. Fekry; Emara, Samir A.; Enayat, E. I.;  
Mustafa, Omnia E. A.  
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt  
SOURCE: Indian Journal of Chemistry, Section B: Organic  
Chemistry Including Medicinal Chemistry (1990),  
29B(9), 811-13  
CODEN: IJSBDB; ISSN: 0376-4699  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Factors affecting cyclization of (benzamide I (R = Me, Ph, PhCH<sub>2</sub>) to the corresponding II were studied. The cyclization process depended on the basicity of the medium, time of reaction, polarity of solvent used as well as the nature of the substituents present.

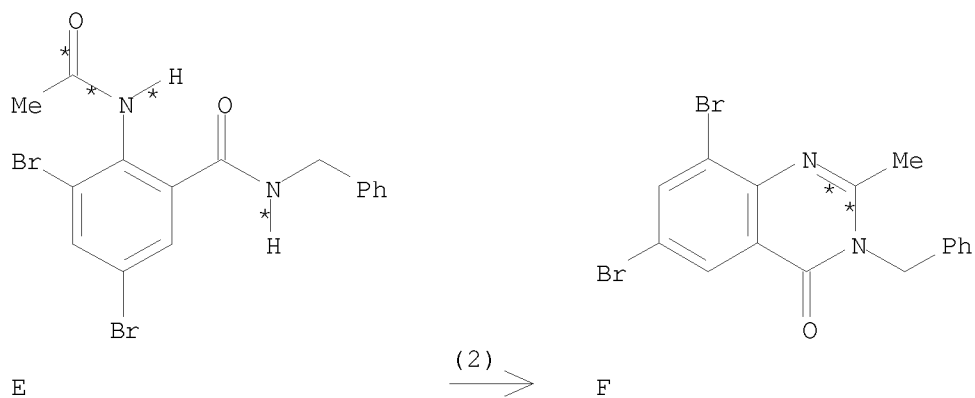
RX(1) OF 3 A ==> B

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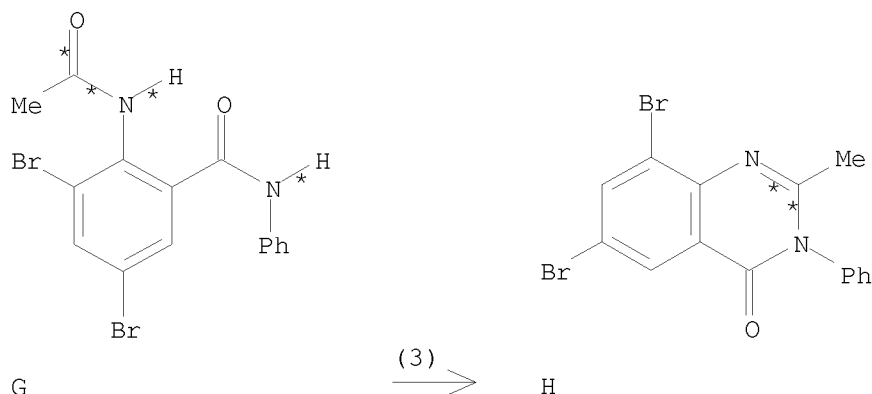
RX(1)      RCT    A 86993-54-6  
              RGT    C 75-04-7 EtNH2  
              PRO    B 86993-61-5  
              SOL    64-17-5 EtOH

RX(2) OF 3      E ==> F



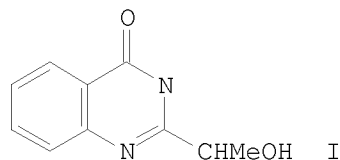
RX(2)      RCT    E 86993-56-8  
              RGT    C 75-04-7 EtNH2  
              PRO    F 86993-63-7  
              SOL    64-17-5 EtOH

RX(3) OF 3      G ==> H



RX(3)      RCT    G 78993-24-5  
              RGT    C 75-04-7 EtNH<sub>2</sub>  
              PRO    H 4145-21-5  
              SOL    64-17-5 EtOH

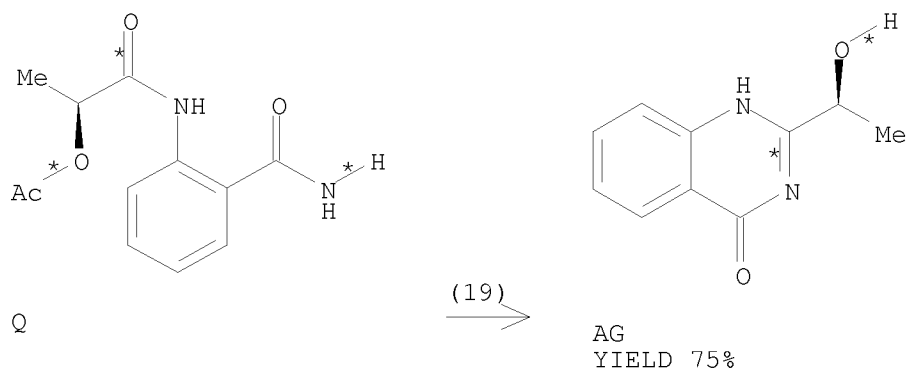
L3    ANSWER 153 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER:      113:171734    CASREACT  
 TITLE:                    Synthesis of chrysogine, a metabolite of *Penicillium*  
                                  chrysogenum and some related 2-substituted  
                                  4-(3H)-quinazolinones  
 AUTHOR(S):                Bergman, Jan; Brynolf, Anna  
 CORPORATE SOURCE:        Dep. Org. Chem., R. Inst. Technol., Stockholm, S-100  
                                  44, Swed.  
 SOURCE:                    Tetrahedron (1990), 46(4), 1295-310  
                                  CODEN: TETRAB; ISSN: 0040-4020  
 DOCUMENT TYPE:            Journal  
 LANGUAGE:                 English  
 GI



AB    Both enantiomers of chrysogine (I) were prepared from 2-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CONH<sub>2</sub> (II). Thus reaction of II and (-)-AcOCHMeCOCl gave (-)-2-AcOCHMeCONHC<sub>6</sub>H<sub>4</sub>CONH<sub>2</sub> which upon saponification and cyclization induced by aqueous Na<sub>2</sub>CO<sub>3</sub> at room temperature gave (S)-(-)-I. The enantiomeric purity of (S)-(-)-I was determined by NMR. Inversion of (-)-(-)-I using the Mitsunobu reaction, gave (+)-(R)-I. Reduction of 2-acetyl-4(3H)-quinazolinone with bakers' yeast gave (S)-(-)-I. The cyclization method could be extended to a number of 2-(α-hydroxy)alkyl-4-(3H)-quinazolinones.

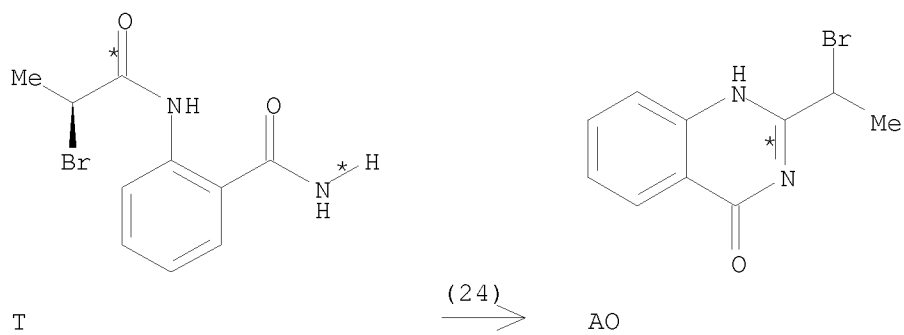
10/ 562,112

RX(19) OF 82 ...Q ==> AG...



RX(19) RCT Q 129768-43-0  
PRO AG 42599-89-3

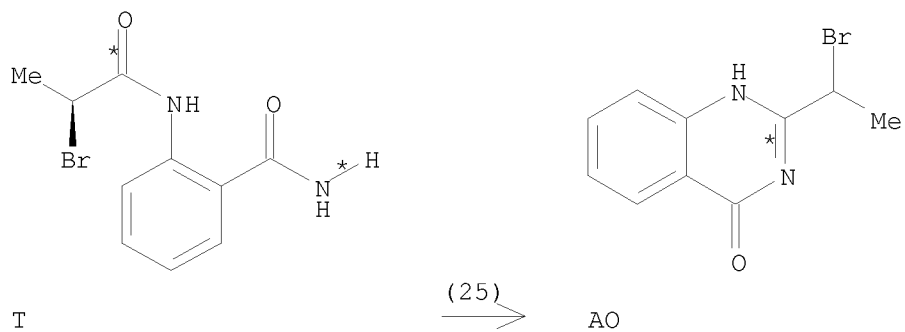
RX(24) OF 82 ...T ==> AO...



RX(24) RCT T 129831-32-9  
PRO AO 144189-81-1  
CAT 104-15-4 TsOH

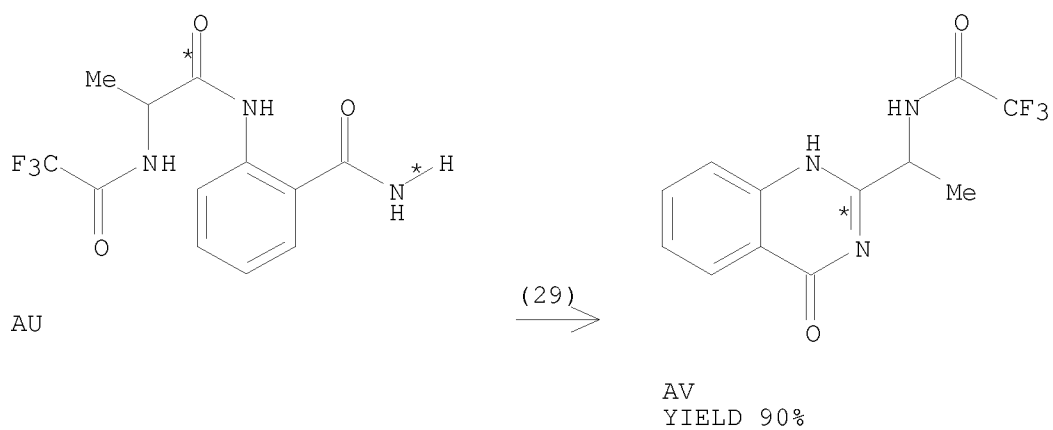
RX(25) OF 82 T ==> AO

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RX(25)      RCT    T 129831-32-9  
             PRO    AO 144189-81-1  
             CAT    497-19-8 Na2CO3

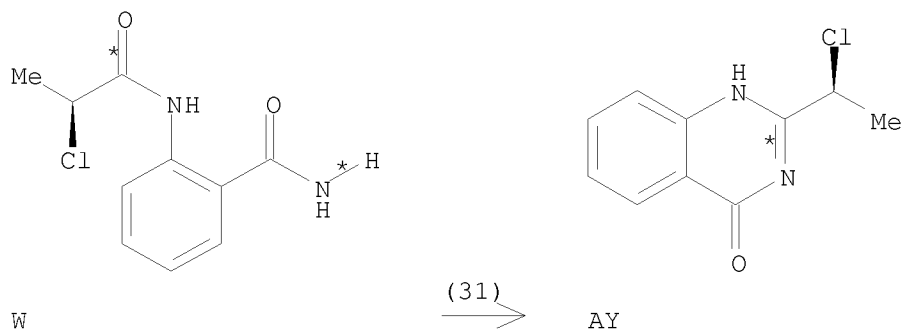
RX(29) OF 82      ...AU    ==>    AV



RX(29)      RCT    AU 129768-61-2  
             PRO    AV 129768-62-3

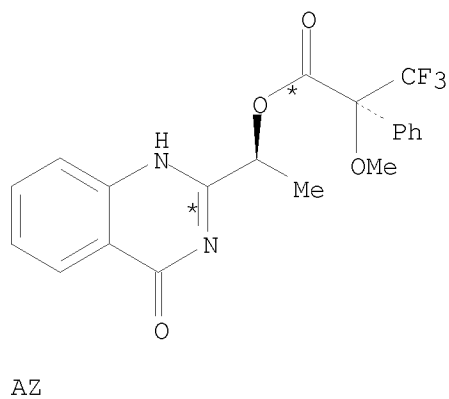
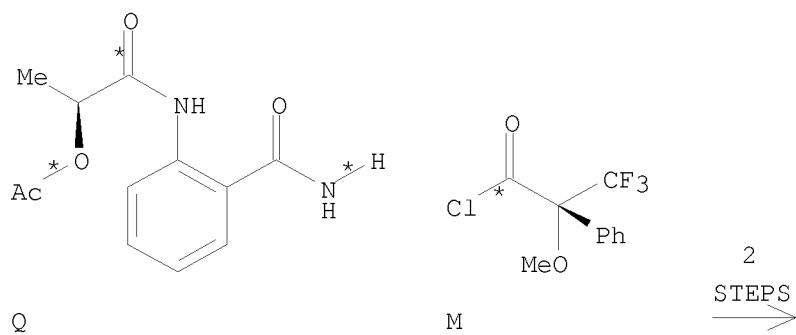
RX(31) OF 82      ...W    ==>    AY

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RX(31) RCT W 129768-48-5  
PRO AY 129768-63-4  
CAT 104-15-4 TsOH

RX(48) OF 82 COMPOSED OF RX(19), RX(32)  
RX(48) Q + M ==> AZ



RX(19) RCT Q 129768-43-0  
PRO AG 42599-89-3

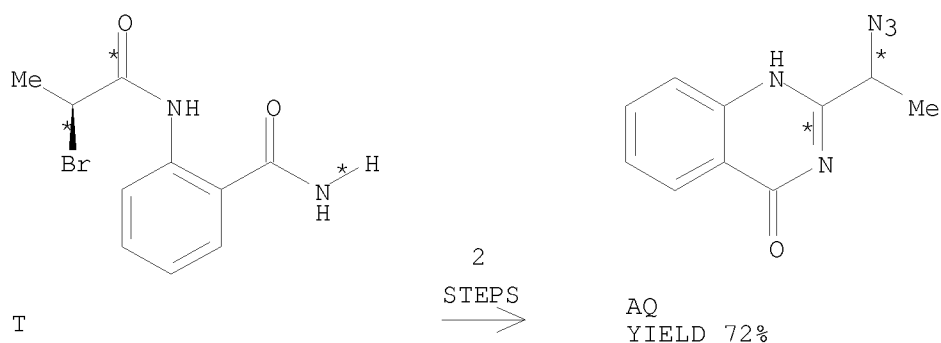


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RX(32)      RCT   AG 42599-89-3, M 20445-33-4  
             PRO   AZ 151163-81-4

RX(51) OF 82 COMPOSED OF RX(24), RX(26)

RX(51)      T      ==>   AQ



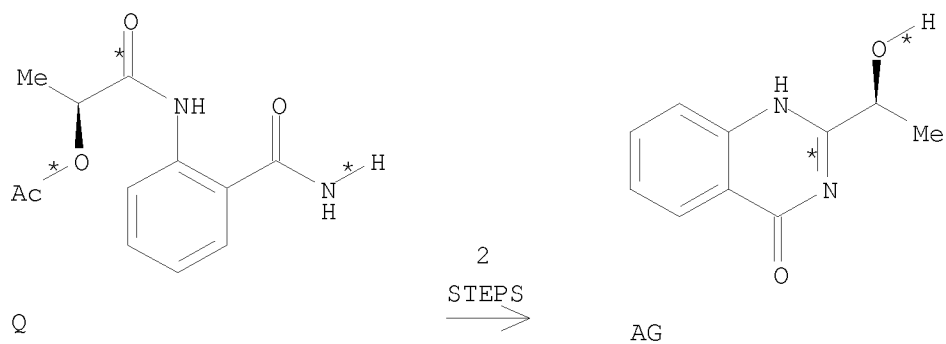
RX(24)      RCT   T 129831-32-9  
             PRO   AO 144189-81-1  
             CAT   104-15-4 TsOH

RX(26)      RCT   AO 144189-81-1  
             RGT   AR 26628-22-8 NaN<sub>3</sub>  
             PRO   AQ 129768-59-8

RX(63) OF 82 COMPOSED OF REACTION SEQUENCE RX(19), RX(32)  
                                 AND REACTION SEQUENCE RX(7), RX(32)

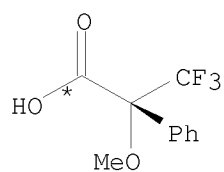
... Q      ==>   AG...

...L + C + AG      ==>   AZ

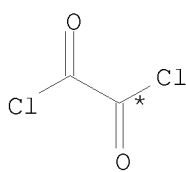


START NEXT REACTION SEQUENCE

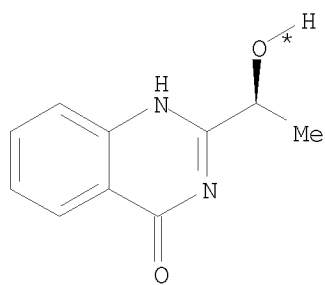
10/ 562,112



L

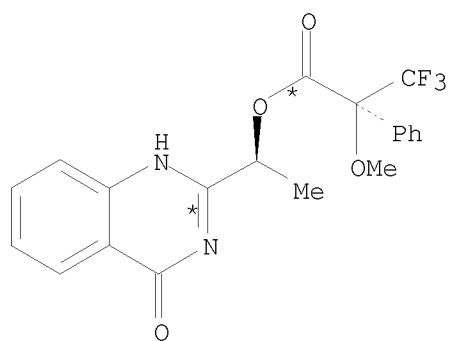


C



AG

2  
STEPS  
→



AZ

RX(19) RCT Q 129768-43-0  
PRO AG 42599-89-3

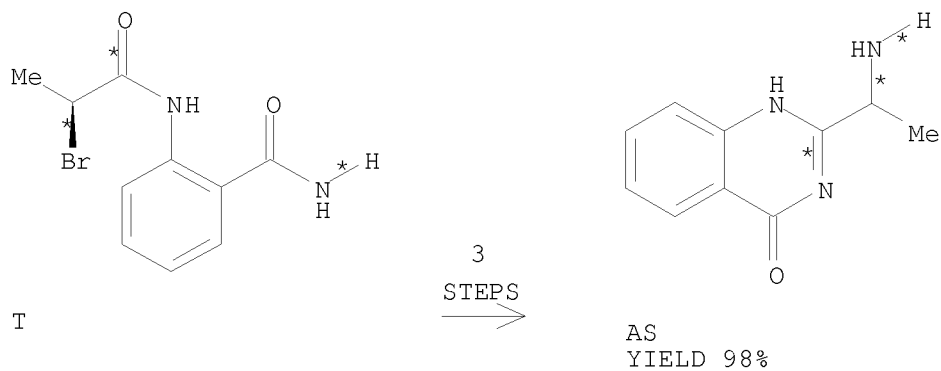
RX(7) RCT L 20445-31-2, C 79-37-8  
PRO M 20445-33-4

RX(32) RCT AG 42599-89-3, M 20445-33-4  
PRO AZ 151163-81-4

RX(72) OF 82 COMPOSED OF RX(24), RX(26), RX(27)

RX(72) T ==> AS

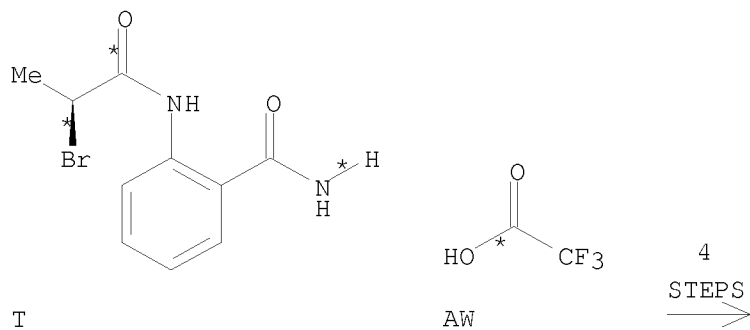
10/ 562,112

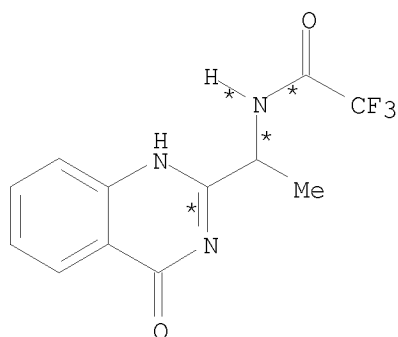


RX(24)	RCT	T 129831-32-9
	PRO	AO 144189-81-1
	CAT	104-15-4 TsOH
RX(26)	RCT	AO 144189-81-1
	RGT	AR 26628-22-8 NaN <sub>3</sub>
	PRO	AQ 129768-59-8
RX(27)	RCT	AQ 129768-59-8
	PRO	AS 172420-42-7

RX(75) OF 82 COMPOSED OF RX(24), RX(26), RX(27), RX(30)

RX(75) T + AW ==> AV





AV

RX(24)	RCT	T 129831-32-9
	PRO	AO 144189-81-1
	CAT	104-15-4 TsOH
RX(26)	RCT	AO 144189-81-1
	RGT	AR 26628-22-8 NaN <sub>3</sub>
	PRO	AQ 129768-59-8
RX(27)	RCT	AQ 129768-59-8
	PRO	AS 172420-42-7
RX(30)	RCT	AS 172420-42-7, AW 76-05-1
	PRO	AV 129768-62-3
	CAT	144-55-8 NaHCO <sub>3</sub>

L3 ANSWER 154 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 113:78293 CASREACT

TITLE: Synthesis and reactions of a  
2-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)oxomethyl-4H-  
3,1-benzoxazin-4-one

AUTHOR(S): Soliman, A. Y.; El-Assy, N. B.; El-Shahed, F.;  
El-Kady, M.; El-Deen, I. M.

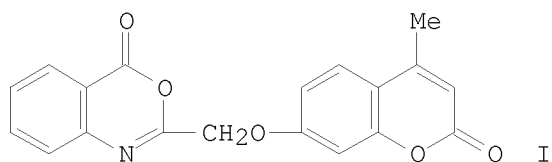
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt

SOURCE: Indian Journal of Chemistry, Section B: Organic  
Chemistry Including Medicinal Chemistry (1990),  
29B(4), 326-30  
CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

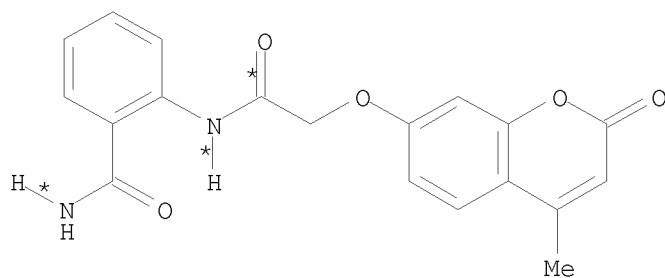
LANGUAGE: English

GI



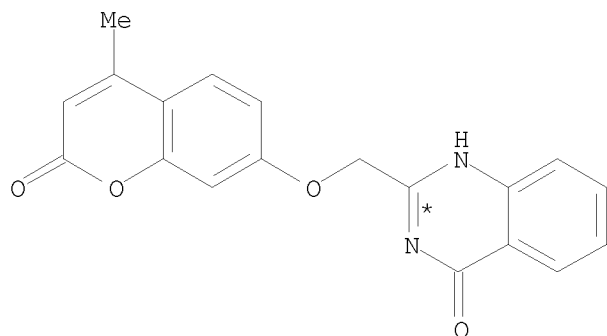
AB The relative reactivity of  $\alpha$ -pyrone and oxazinone rings in 2-(4-methyl-2-oxo-2H-1-benzopyran-7-yloxomethyl)-4H-3,1-benzoxazin-4-one (I) towards nucleophiles (arylation under Friedel Crafts conditions, aminolysis and hydrazinolysis) and electrophiles (aromatic aldehydes) has been described.

RX(17) OF 128 ...AJ ==> AM



AJ

(17)  $\longrightarrow$

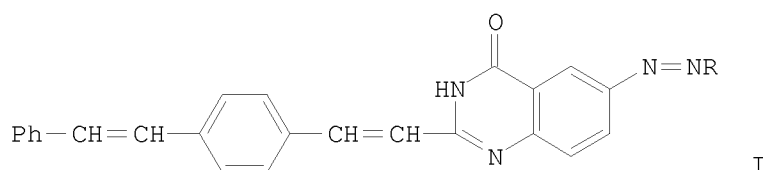


AM

RX(17)    RCT    AJ 128649-83-2  
           RGT    AN 108-24-7 Ac2O  
           PRO    AM 128649-84-3

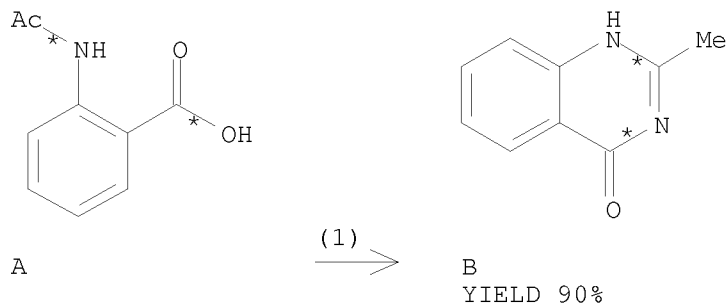
10/ 562,112

L3 ANSWER 155 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 113:42449 CASREACT  
TITLE: Synthesis of azo disperse dyes from 2-(bis  
styryl)-6-amino-4-oxoquinazoline and their application  
on polyester fibers  
AUTHOR(S): Naik, N. M.; Desai, K. R.  
CORPORATE SOURCE: Dep. Chem., South Gujarat Univ., Surat, 395 007, India  
SOURCE: Indian Journal of Textile Research (1989), 14(4),  
184-6  
CODEN: IJTRDU; ISSN: 0377-8436  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB The title dyes (I; R = from Naphthol AS, AS-G, AS-D, AS-E, AS-BS, AS-OL, AS-BO, or AS-SW, or BON acid) were synthesized by azo coupling and color and fastness properties of I on polyester fabrics were determined

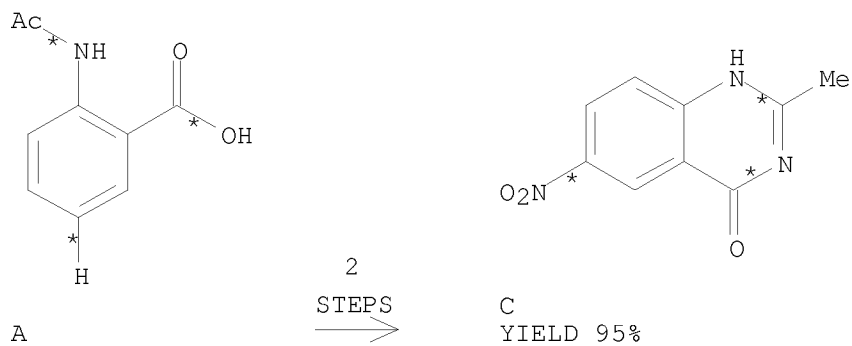
RX(1) OF 21 A ==> B...



RX(1) RCT A 89-52-1  
PRO B 1769-24-0

RX(7) OF 21 COMPOSED OF RX(1), RX(2)  
RX(7) A ==> C

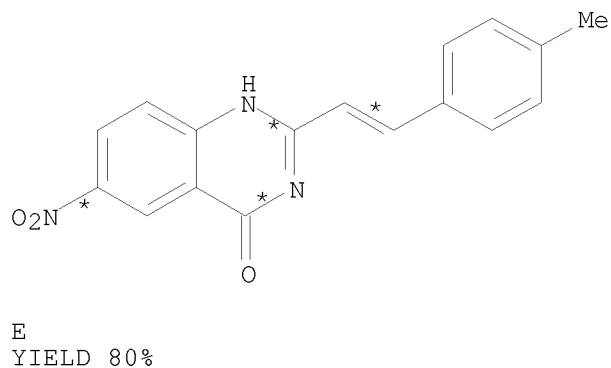
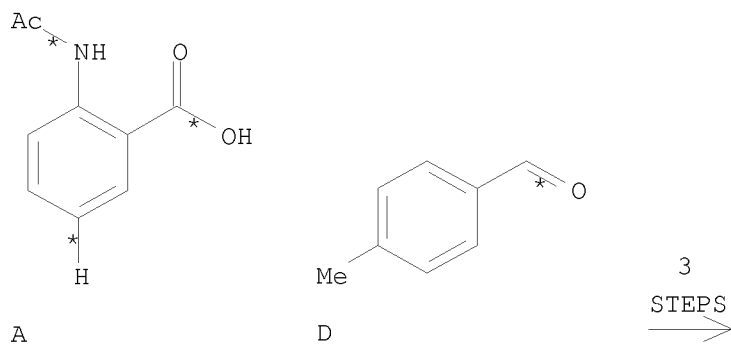
10/ 562,112



RX(1) RCT A 89-52-1  
PRO B 1769-24-0

RX(2) RCT B 1769-24-0  
PRO C 24688-36-6

RX(12) OF 21 COMPOSED OF RX(1), RX(2), RX(3)  
RX(12) A + D ==> E



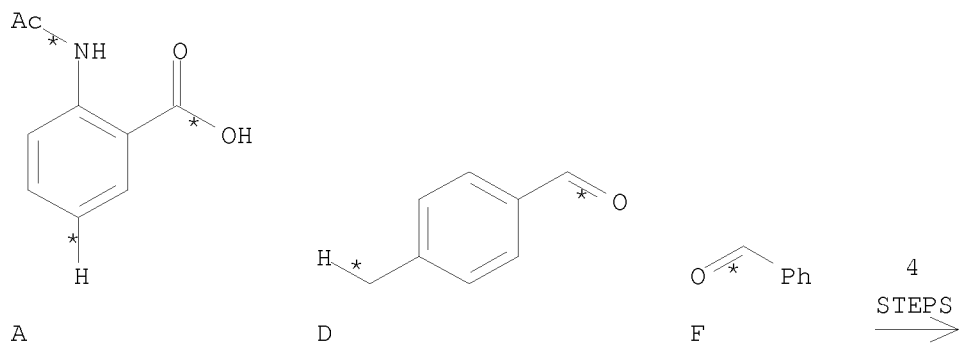
RX(1) RCT A 89-52-1  
PRO B 1769-24-0

10/ 562,112

RX(2) RCT B 1769-24-0  
PRO C 24688-36-6

RX(3) RCT C 24688-36-6, D 104-87-0  
PRO E 73673-70-8

RX(14) OF 21 COMPOSED OF RX(1), RX(2), RX(3), RX(4)  
RX(14) A + D + F ==> G



G  
YIELD 83%

RX(1) RCT A 89-52-1  
PRO B 1769-24-0

RX(2) RCT B 1769-24-0  
PRO C 24688-36-6

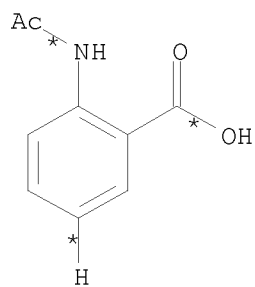
RX(3) RCT C 24688-36-6, D 104-87-0  
PRO E 73673-70-8

RX(4) RCT E 73673-70-8, F 100-52-7  
PRO G 128031-42-5

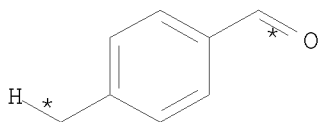
RX(19) OF 21 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5)  
RX(19) A + D + F ==> H



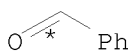




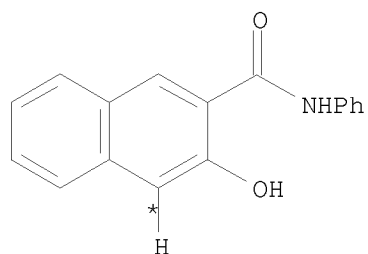
A



D

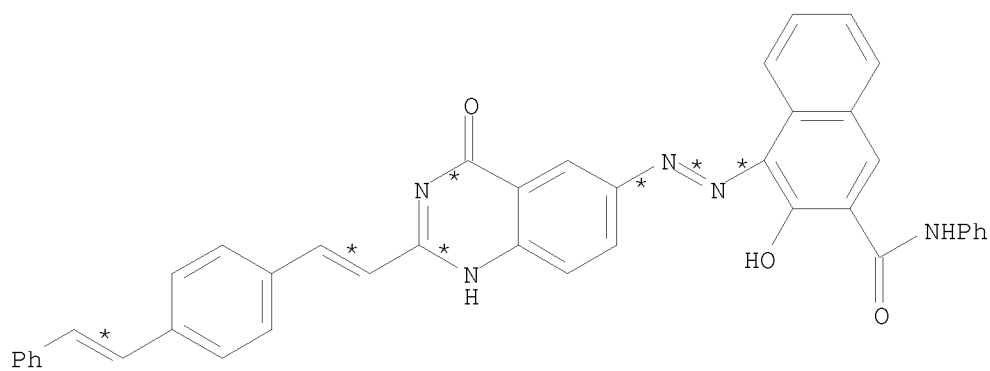


F



I

6  
STEPS  
→



J

YIELD 76%

RX(1) RCT A 89-52-1  
PRO B 1769-24-0

RX(2) RCT B 1769-24-0  
PRO C 24688-36-6

RX(3) RCT C 24688-36-6, D 104-87-0  
PRO E 73673-70-8

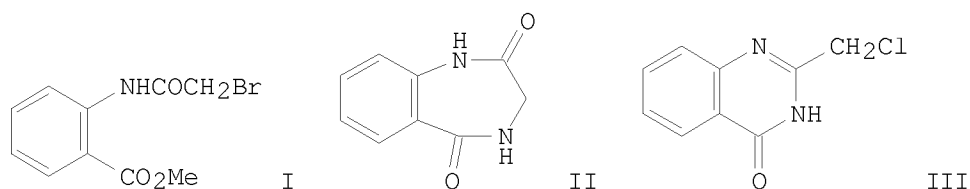
10/ 562,112

RX(4) RCT E 73673-70-8, F 100-52-7  
PRO G 128031-42-5

RX(5) RCT G 128031-42-5  
PRO H 128031-43-6

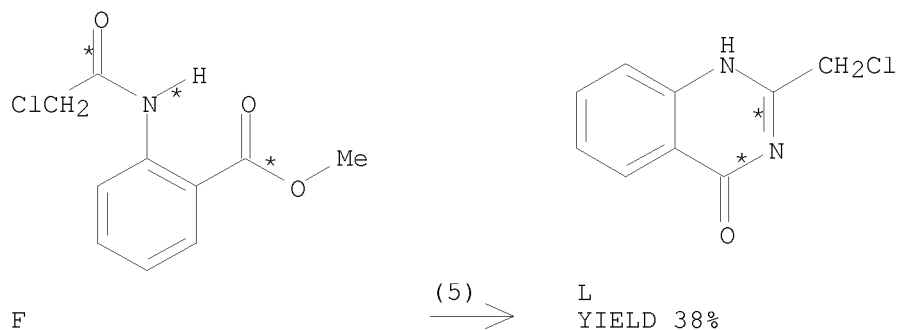
RX(6) RCT H 128031-43-6, I 92-77-3  
PRO J 128031-35-6

L3 ANSWER 156 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 113:40636 CASREACT  
TITLE: Ring closure reactions of methyl  
N-(haloacetyl)anthranilates with ammonia  
AUTHOR(S): Cho, Nam Sook; Song, Ki Youn; Parkanyi, Cyril  
CORPORATE SOURCE: Dep. Chem., Chungnam Natl. Univ., Daejeon, 302-764, S.  
Korea  
SOURCE: Journal of Heterocyclic Chemistry (1989), 26(6),  
1807-10  
CODEN: JHTCAD; ISSN: 0022-152X  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



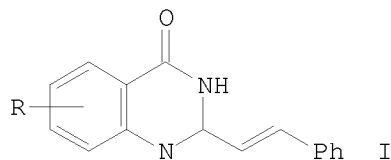
AB In the presence of ammonia, Me N-(bromoacetyl)anthranilate (I) is cyclized into 3H-1,4-benzodiazepine-2,5(1H,4H)-dione (II). However, when I is replaced with Me N-(chloroacetyl)anthranilate, the only heterocyclic product formed in the reaction is 2-(chloromethyl)quinazoline-4(3H)-one (III). Under analogous conditions, 3-haloacetamidocrotonates  $RCH_2CONHCHMe:CHCO_2Et$  ( $R = Br, Cl$ ) do not yield any heterocyclic products and no 1,4-diazepines can be obtained.

RX(5) OF 11 ...F ==> L



RX(5)      RCT   F 58915-18-7  
              RGT   I 7664-41-7 NH3  
              PRO   L 3817-05-8  
              SOL   67-56-1 MeOH

L3    ANSWER 157 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER:    112:235257    CASREACT  
 TITLE:    Synthesis and biological evaluation of  
              2-styrylquinazolin-4(3H)-ones, a new class of  
              antimitotic anticancer agents which inhibit tubulin  
              polymerization  
 AUTHOR(S):    Jiang, Jack B.; Hesson, D. P.; Dusak, B. A.; Dexter,  
                      D. L.; Kang, G. J.; Hamel, E.  
 CORPORATE SOURCE:    E. I. Du Pont de Nemours and Co., Wilmington, DE,  
                                  19880, USA  
 SOURCE:    Journal of Medicinal Chemistry (1990), 33(6), 1721-8  
                  CODEN: JMCMAR; ISSN: 0022-2623  
 DOCUMENT TYPE:    Journal  
 LANGUAGE:    English  
 GI

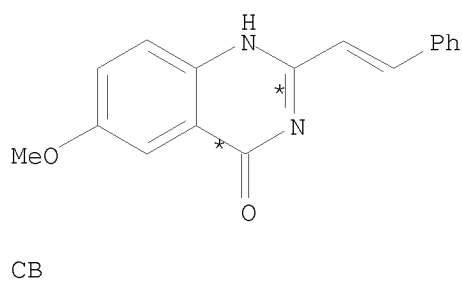
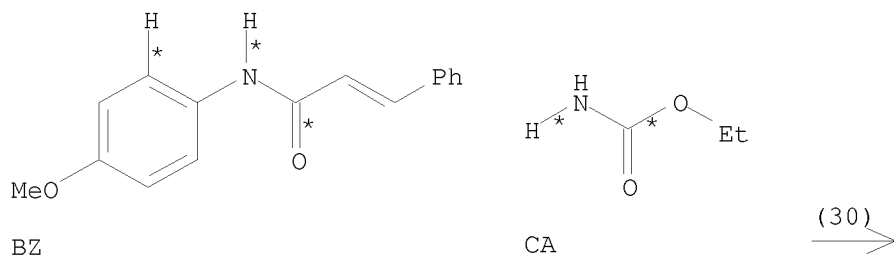


AB    Title compds., e.g., I (R = 5-, 6-, 7-, 8-Cl, 6-Br, 6-F, 6-NH<sub>2</sub>, 6-OMe, 5-,  
 6-Me, 6-OH, 6-OEt) were prepared. Extensive structure-activity relationship  
 studies suggest that the entire quinazolinone structure was required, but  
 activity was further enhanced by halide or small hydrophobic substituents  
 at position 6. These analogs did not substantially interfere with the  
 binding of radiolabeled colchicine, vinblastine, or GTP to tubulin and  
 weakly stimulated GTP hydrolysis uncoupled from polymerization. Several analogs  
 have shown in vivo tumor growth inhibitory activity in the L1210 leukemia  
 model, with the lead compound I (R = 6-OMe) exhibiting good antitumor

10/ 562,112

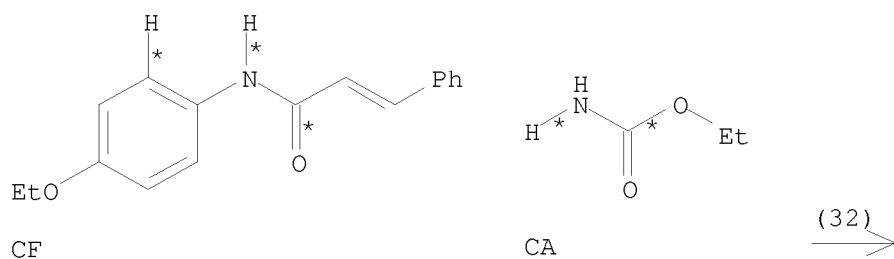
activity against murine solid tumors as well as human tumor xenografts.

RX(30) OF 64      BZ + CA ==> CB...

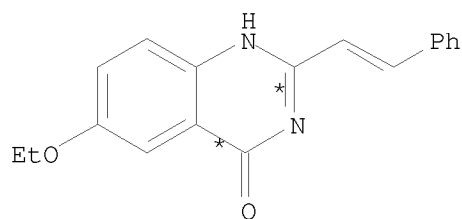


RX(30)      RCT    BZ 76228-15-4, CA 51-79-6  
             RGT    AW 1314-56-3 P205  
             PRO    CB 127033-41-4  
             SOL    1330-20-7 Xylene

RX(32) OF 64      CF + CA ==> CG



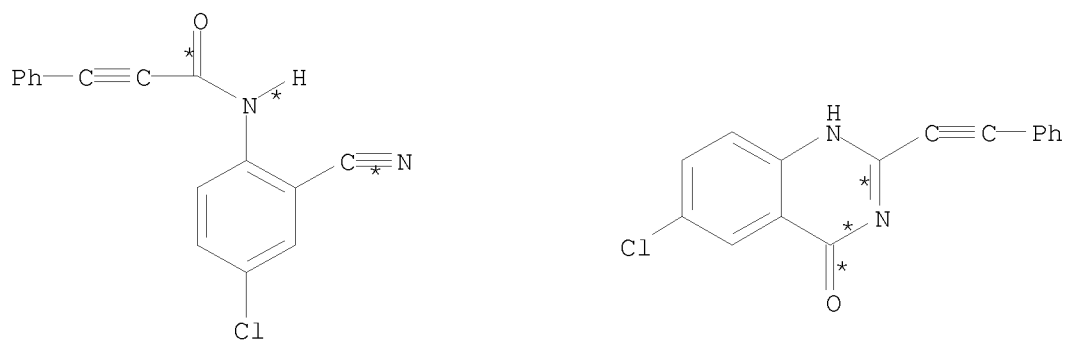
10/ 562,112



CG

RX(32)     RCT   CF 127033-73-2, CA 51-79-6  
           RGT   AW 1314-56-3 P2O5  
           PRO   CG 127033-44-7  
           SOL   1330-20-7 Xylene

RX(39) OF 64     CQ   ==>   CR



CQ

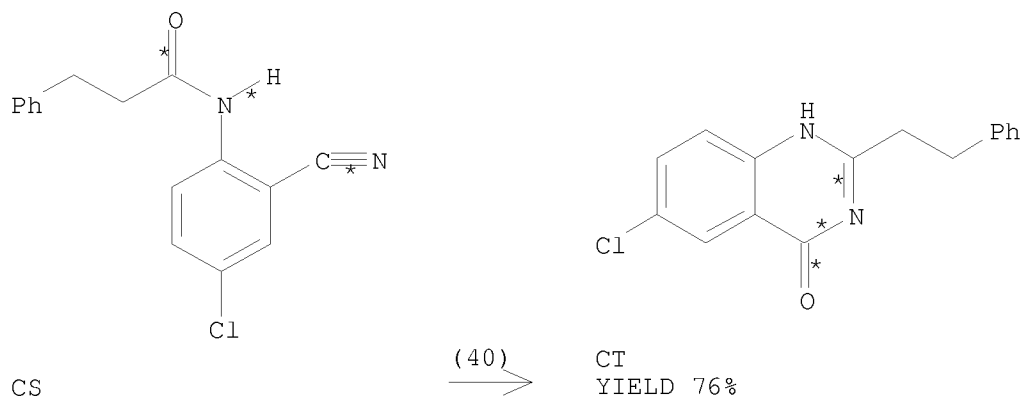
(39)  $\longrightarrow$

CR  
YIELD 18%

RX(39)     RCT   CQ 127033-75-4  
           RGT   E 1310-73-2 NaOH, F 7722-84-1 H2O2  
           PRO   CR 127033-55-0  
           SOL   64-17-5 EtOH, 7732-18-5 Water

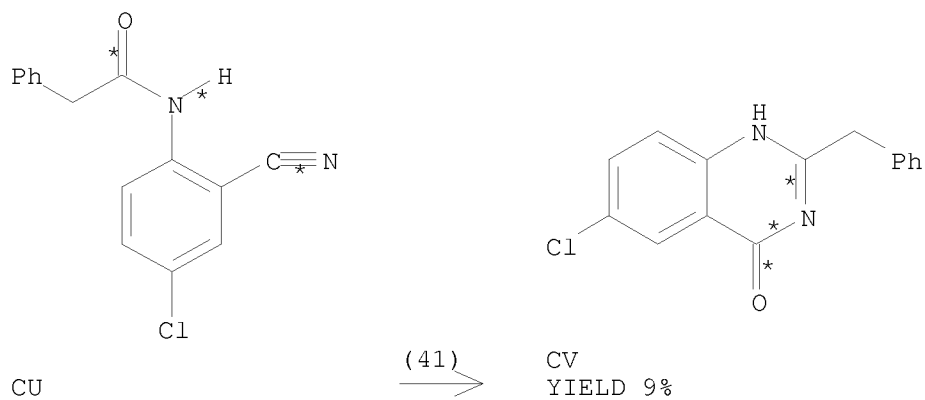
RX(40) OF 64     CS   ==>   CT

10/ 562,112



RX(40) RCT CS 127033-76-5  
RGT E 1310-73-2 NaOH, F 7722-84-1 H2O2  
PRO CT 127033-56-1  
SOL 64-17-5 EtOH, 7732-18-5 Water

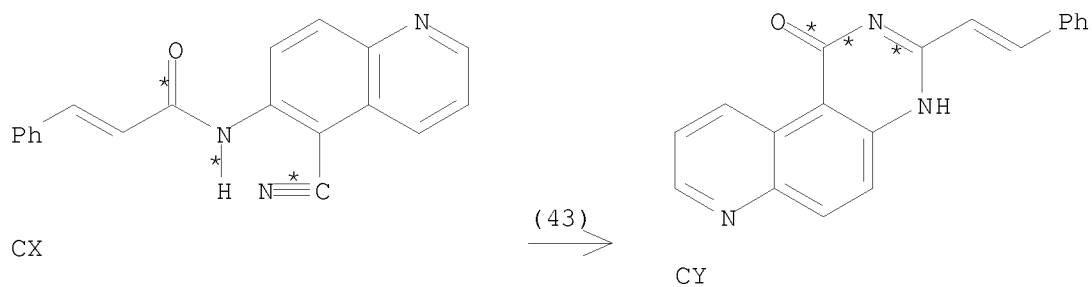
RX(41) OF 64 CU  $\implies$  CV



RX(41) RCT CU 127033-77-6  
RGT E 1310-73-2 NaOH, F 7722-84-1 H2O2  
PRO CV 35834-17-4  
SOL 64-17-5 EtOH, 7732-18-5 Water

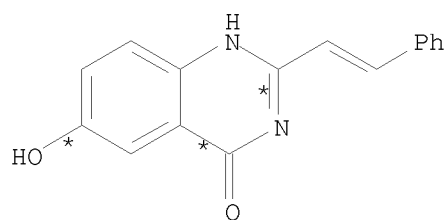
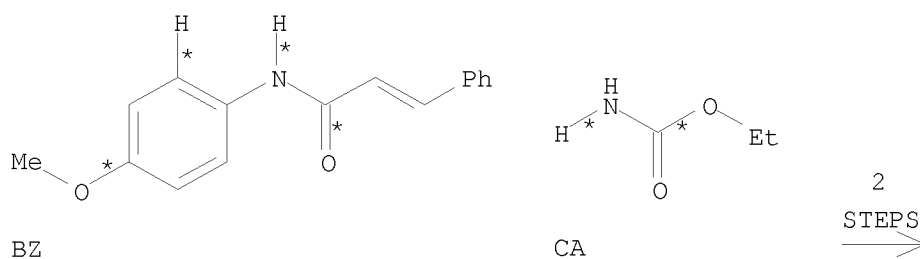
RX(43) OF 64 CX  $\implies$  CY

10/ 562,112



RX(43) RCT CX 127033-78-7  
 RGT E 1310-73-2 NaOH, F 7722-84-1 H2O2  
 PRO CY 127033-70-9  
 SOL 64-17-5 EtOH, 7732-18-5 Water

RX(58) OF 64 COMPOSED OF RX(30), RX(31)  
 RX(58) BZ + CA ==> CD



CD  
 YIELD 63%

RX(30) RCT BZ 76228-15-4, CA 51-79-6  
 RGT AW 1314-56-3 P2O5  
 PRO CB 127033-41-4  
 SOL 1330-20-7 Xylene

RX(31) RCT CB 127033-41-4  
 RGT CE 10035-10-6 HBr  
 PRO CD 127033-42-5  
 SOL 7732-18-5 Water, 64-19-7 AcOH



L3 ANSWER 158 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 112:216853 CASREACT

TITLE: Synthesis and rearrangement of  
4-imino-4H-3,1-benzoxazines

AUTHOR(S): Mazurkiewicz, Roman

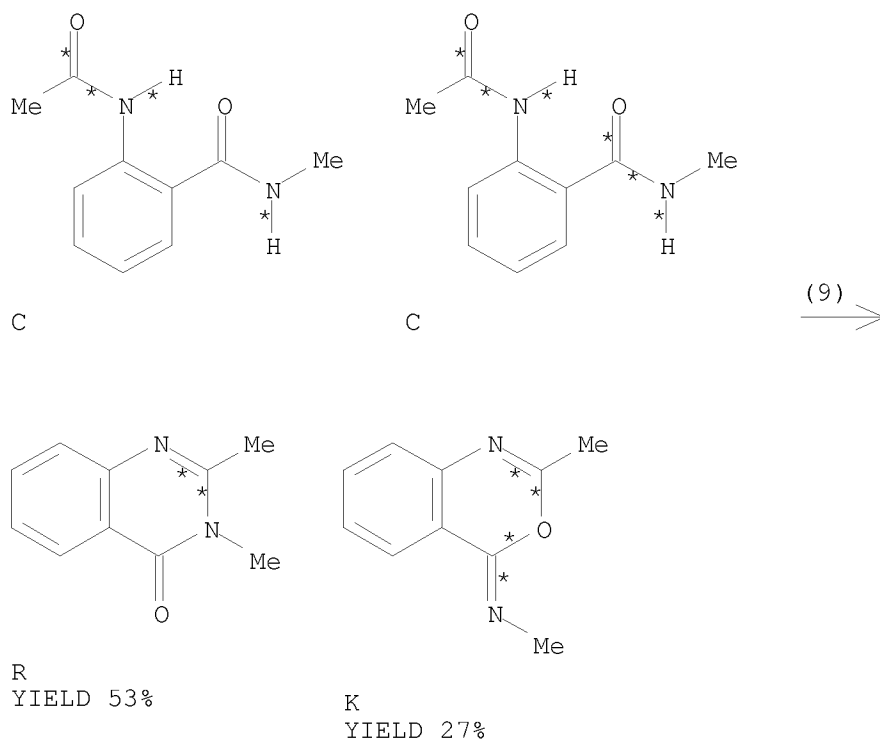
CORPORATE SOURCE: Inst. Org. Chem. Technol., Silesian Tech. Univ.,  
Gliwice, PL-44-101, Pol.SOURCE: Monatshefte fuer Chemie (1989), 120(11), 973-80  
CODEN: MOCMB7; ISSN: 0026-9247

DOCUMENT TYPE: Journal

LANGUAGE: English

AB o-RNHCOC6H4NHCOR1 (I; R, R1 = Me, Ph) react with Ph3P-Br in the presence of Et3N as HBr captor to give 2-methyl- or 2-phenyl-4-imino-4H-3,1-benzoxazines in good yields. Without an acid acceptor, I (R1 = Me) yield 2-methyl-4-quinazolones, while I (R1 = Ph) give 2-phenyl-4-imino-4H-3,1-benzoxazines. 2-Methyl-4-imino-4H-3,1-benzoxazines rearrange under the influence of HCl or HBr into the resp. 2-methyl-4-quinazolones; the 2-phenyl analogs, however, do not rearrange.

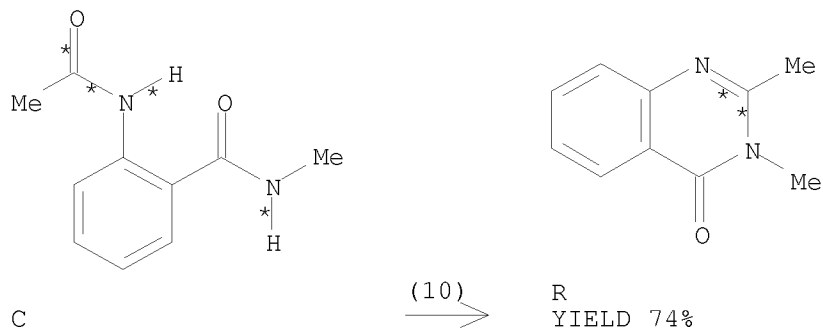
RX(9) OF 24 ...2 C ==&gt; R + K...



RX(9) RCT C 59525-16-5  
RGT L 7726-95-6 Br2, S 7446-70-0 AlCl3  
PRO R 1769-25-1, K 127082-55-7  
SOL 75-09-2 CH2Cl2

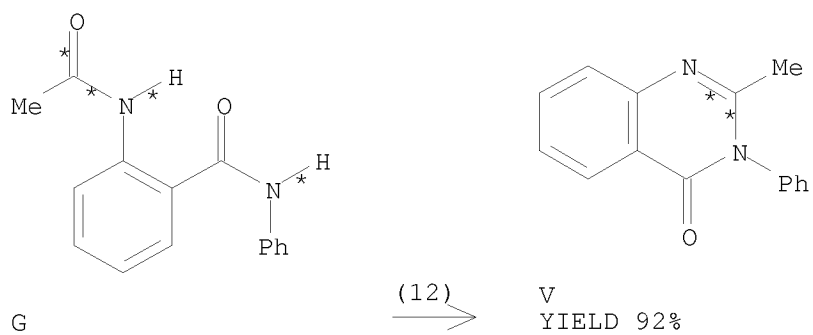
10/ 562,112

RX(10) OF 24 ...C ==> R



RX(10) RCT C 59525-16-5  
RGT L 7726-95-6 Br<sub>2</sub>, S 7446-70-0 AlCl<sub>3</sub>  
PRO R 1769-25-1  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

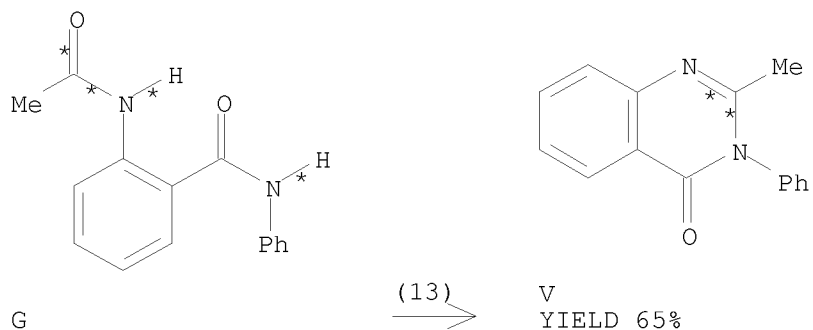
RX(12) OF 24 ...G ==> V



RX(12) RCT G 54364-31-7  
RGT T 7647-01-0 HCl  
PRO V 2385-23-1  
SOL 107-06-2 ClCH<sub>2</sub>CH<sub>2</sub>Cl

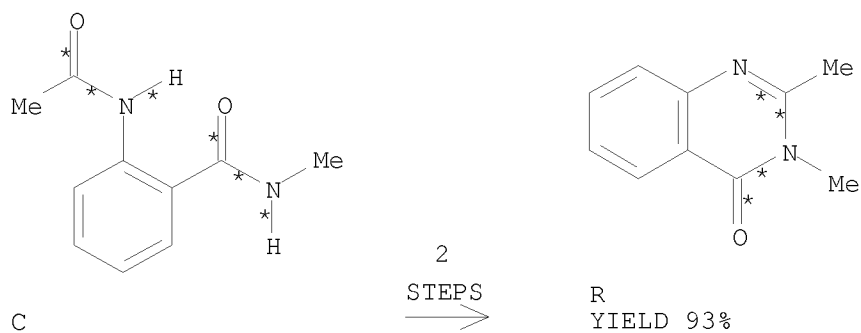
RX(13) OF 24 G ==> V

10/ 562,112



RX(13) RCT G 54364-31-7  
RGT L 7726-95-6 Br<sub>2</sub>, S 7446-70-0 AlCl<sub>3</sub>  
PRO V 2385-23-1  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

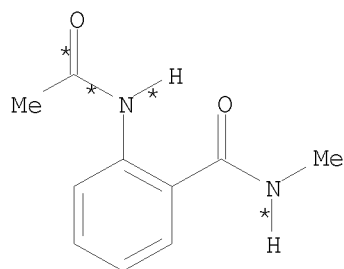
RX(21) OF 24 COMPOSED OF RX(5), RX(11)  
RX(21) C ==> R



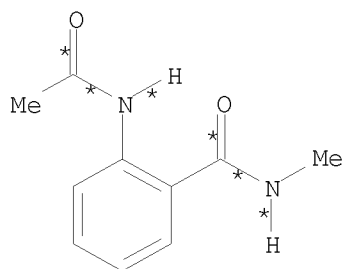
RX(5) RCT C 59525-16-5  
RGT L 7726-95-6 Br<sub>2</sub>, M 603-35-0 PPh<sub>3</sub>, D 121-44-8 Et<sub>3</sub>N  
PRO K 127082-55-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(11) RCT K 127082-55-7  
RGT T 7647-01-0 HCl  
PRO R 1769-25-1  
SOL 107-06-2 ClCH<sub>2</sub>CH<sub>2</sub>Cl

RX(22) OF 24 COMPOSED OF RX(9), RX(11)  
RX(22) 2 C ==> R

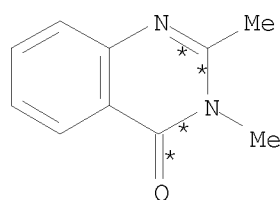


C



C

2  
STEPS  
→



R  
YIELD 93%

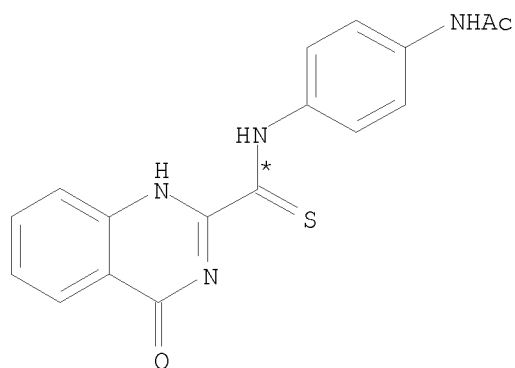
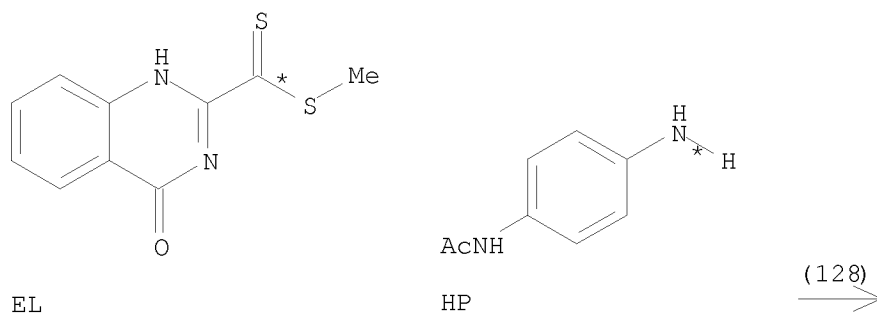
RX(9) RCT C 59525-16-5  
RGT L 7726-95-6 Br<sub>2</sub>, S 7446-70-0 AlCl<sub>3</sub>  
PRO R 1769-25-1, K 127082-55-7  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(11) RCT K 127082-55-7  
RGT T 7647-01-0 HCl  
PRO R 1769-25-1  
SOL 107-06-2 ClCH<sub>2</sub>CH<sub>2</sub>Cl

L3 ANSWER 159 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 112:157325 CASREACT  
TITLE: Dithiocarboxylic acids, dithiocarboxylic esters, or  
thiocarboxylic amides by reaction of methylene-active  
chloromethyl compounds with sulfur  
AUTHOR(S): Thiel, W.; Mayer, R.  
CORPORATE SOURCE: Sekt. Chem., Tech. Univ. Dresden, Dresden, DDR-8027,  
Ger. Dem. Rep.  
SOURCE: Journal fuer Praktische Chemie (Leipzig) (1989),  
331(2), 243-62  
CODEN: JPCEAO; ISSN: 0021-8383  
DOCUMENT TYPE: Journal  
LANGUAGE: German  
AB With a mixture of S and amine in DMF at room temperature halomethyl compds.  
can be oxidized to give thiocarboxylic acids and their derivs. The reaction was  
studied in detail especially with chloroacetic derivs. or chloromethyl

heterocycles formally derived from chloroacetic acid. The resulting thiooxalic acid derivs. represent activated acids and very useful C2-synthons, especially for the synthesis of heterocycles. Oxidation in the presence of Et3N leads to dithiocarboxylates which can be alkylated to dithioesters in high yields. As a rule, with different primary and secondary amines instead of tertiary amines these dithiocarboxylates or dithiocarboxylic esters can be transformed already at low temps. to thioamides.

RX(128) OF 251 ...EL + HP ==> HU

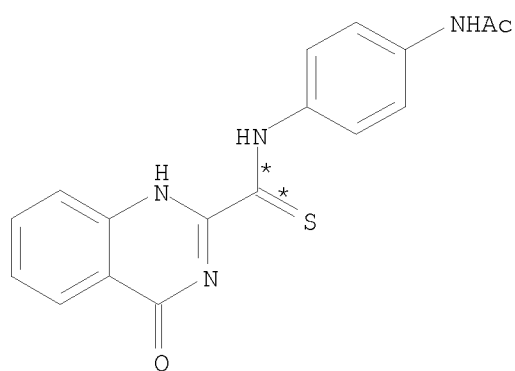
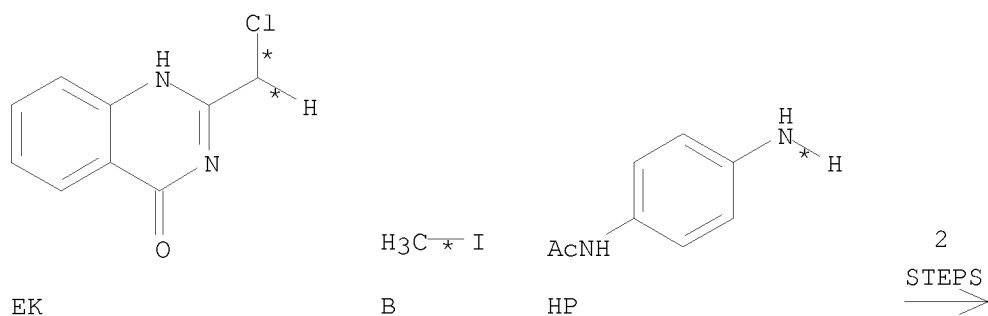


HU  
YIELD 75%

RX(128) RCT EL 125983-30-4, HP 122-80-5  
PRO HU 125983-51-9  
SOL 64-17-5 EtOH

RX(247) OF 251 COMPOSED OF RX(74), RX(128)  
RX(247) EK + B + HP ==> HU

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HU  
YIELD 75%

RX(74) RCT EK 3817-05-8

STAGE(1)

RGT D 7704-34-9 S, E 121-44-8 Et3N

SOL 68-12-2 DMF

STAGE(2)

RCT B 74-88-4

PRO EL 125983-30-4

RX(128) RCT EL 125983-30-4, HP 122-80-5

PRO HU 125983-51-9

SOL 64-17-5 EtOH

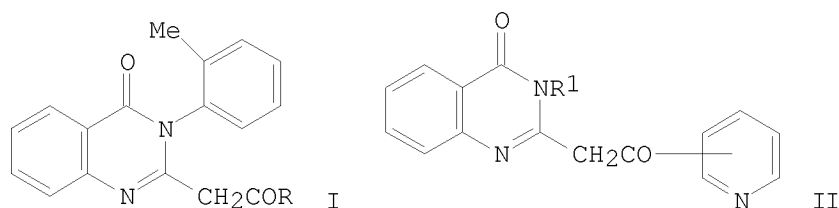
L3 ANSWER 160 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 112:35794 CASREACT

TITLE: Synthesis and anticonvulsant activity of some new  
2-substituted 3-aryl-4(3H)-quinazolinones

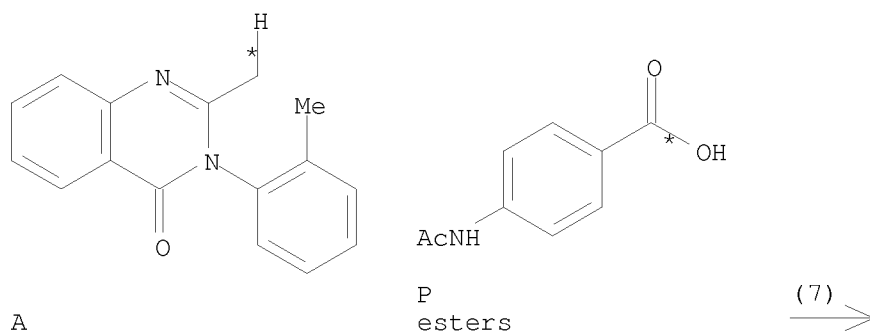
AUTHOR(S): Wolfe, James F.; Rathman, Terry L.; Sleevi, Mark C.;  
Campbell, James A.; Greenwood, Thomas D.

CORPORATE SOURCE: Dep. Chem., Virginia Polytech. Inst. and State Univ., Blacksburg, VA, 24061, USA  
 SOURCE: Journal of Medicinal Chemistry (1990), 33(1), 161-6  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

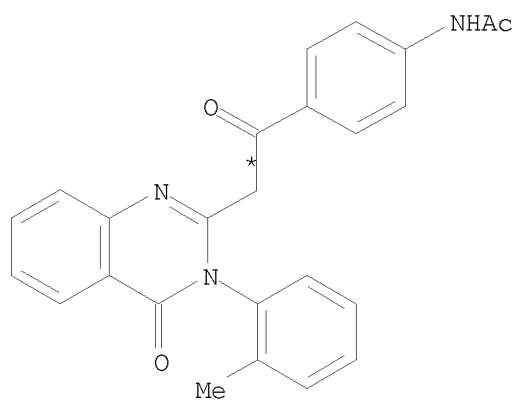


AB 4(3H)-Quinazolinones I (R = Me, Ph, 1-adamantyl, etc.) and II [R1 = (un)substituted Ph], structurally related to methaqualone were synthesized and evaluated for anticonvulsant activity. E.g., treating methaqualone with  $\text{RCO}_2\text{R}_1$  (R1 = ester group) in the presence of NaH gave I. Preliminary screening of these compds. revealed that I (R = 2-pyridyl) (III) and II [o-ClC<sub>6</sub>H<sub>4</sub> (IV), o-BrC<sub>6</sub>H<sub>4</sub>, o-FC<sub>6</sub>H<sub>4</sub>, o-MeOC<sub>6</sub>H<sub>4</sub>, o-IC<sub>6</sub>H<sub>4</sub>] having a single ortho substituent on the 3-aryl group had the most promising anticonvulsant activity. III and IV possessing 3-o-tolyl and 3-o-chlorophenyl groups, resp., showed good protection against maximum electroshock- and s.c. metrazol-induced seizures, combined with relatively low neurotoxicity after i.p. administration in mice. They also exhibited low toxicity in tests for determining the mean hypnotic dose (HD<sub>50</sub>) and the median LD (LD<sub>50</sub>). Although these compds. were markedly more potent as anticonvulsants when administered orally in mice and rats, they were also more neurotoxic. This neurotoxicity was particularly acute in oral tests with rats, which resulted in marginal protective indexes. In drug differentiation tests, III was ineffective against seizures induced by bicuculline, picrotoxin, and strychnine, while IV showed some protection against picrotoxin-induced seizures.

RX(7) OF 73 ...A + P ==> Q



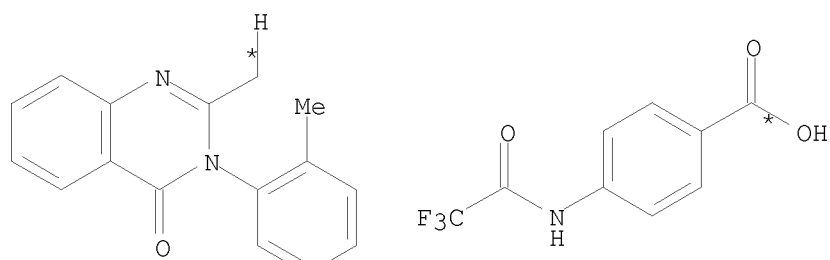
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Q  
YIELD 42%

RX(7) RCT A 72-44-6, P 556-08-1D  
RGT D 7646-69-7 NaH  
PRO Q 73283-19-9  
SOL 109-99-9 THF

RX(8) OF 73 ...A + S ==> T



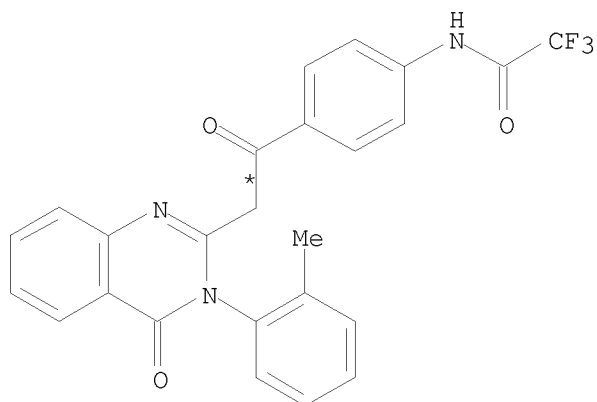
A

S  
esters

(8)  $\longrightarrow$



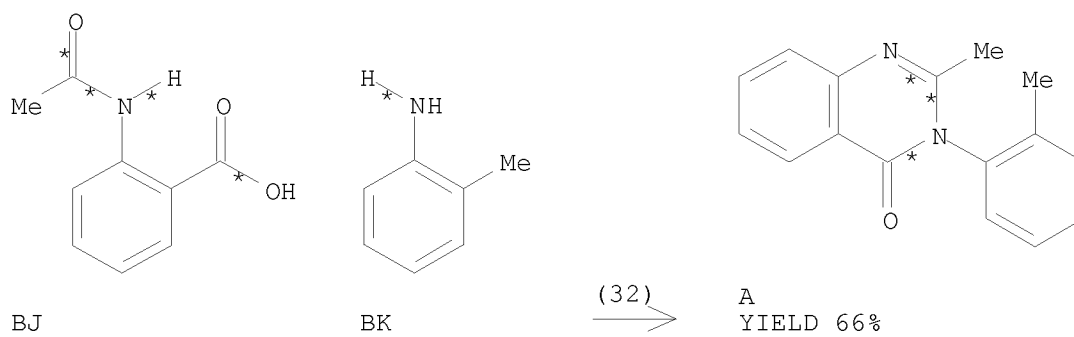
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T  
YIELD 47%

RX(8)	RCT	A 72-44-6, S 404-26-2D
	RGT	D 7646-69-7 NaH
	PRO	T 73283-18-8
	SOL	109-99-9 THF

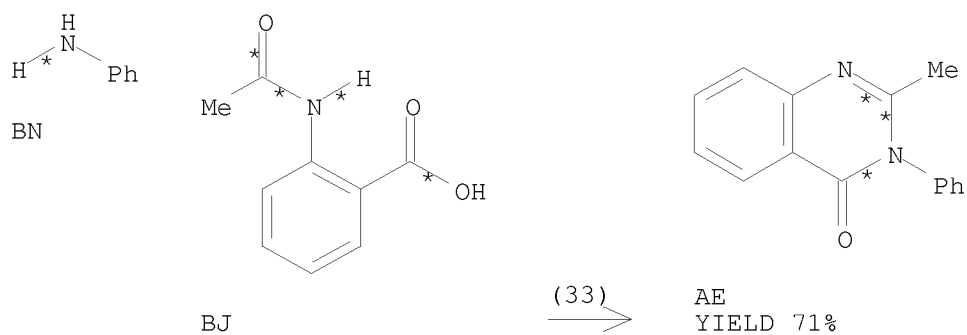
RX(32) OF 73      BJ   +   BK   ==>   A...



RX(32)      RCT    BJ 89-52-1, BK 95-53-4  
               RGT    BL 7719-12-2 PC13  
               PRO    A 72-44-6  
               SOL    108-88-3 PhMe

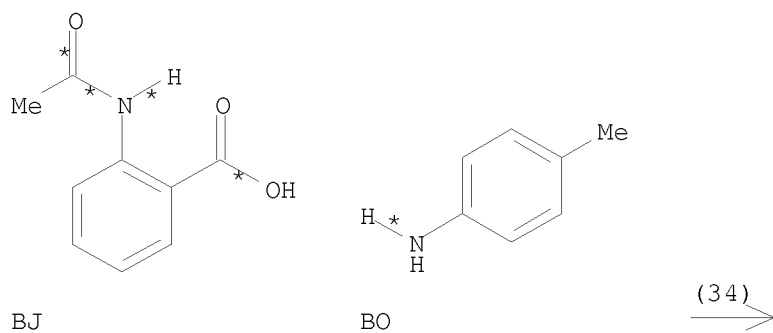
RX(33) OF 73      BN + BJ ==&gt; AE...

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RX(33) RCT BN 62-53-3, BJ 89-52-1  
RGT BL 7719-12-2 PC13  
PRO AE 2385-23-1  
SOL 108-88-3 PhMe

RX(34) OF 73 BJ + BO ==> AL...

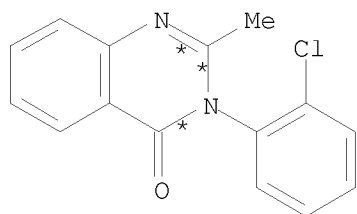
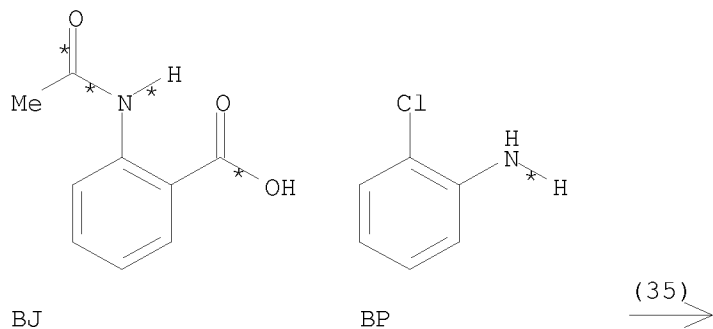


AL  
YIELD 77%

RX(34) RCT BJ 89-52-1, BO 106-49-0  
RGT BL 7719-12-2 PC13  
PRO AL 22316-59-2  
SOL 108-88-3 PhMe

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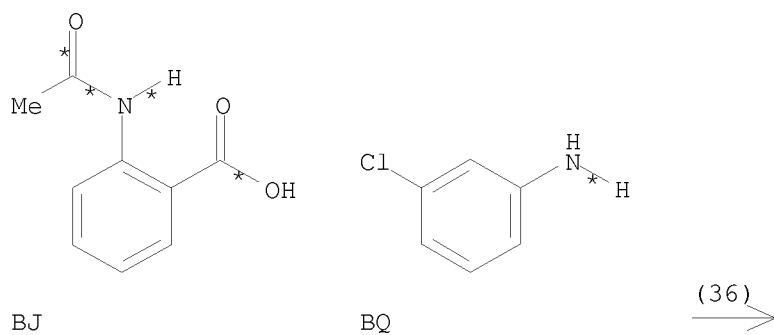
RX(35) OF 73      BJ + BP ==> AP...



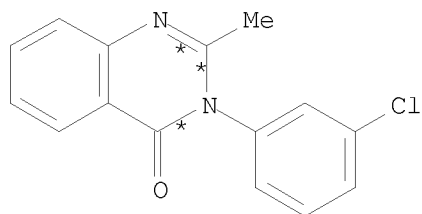
AP  
YIELD 62%

RX(35)      RCT    BJ 89-52-1, BP 95-51-2  
             RGT    BL 7719-12-2 PC13  
             PRO    AP 340-57-8  
             SOL    108-88-3 PhMe

RX(36) OF 73      BJ + BQ ==> AT...



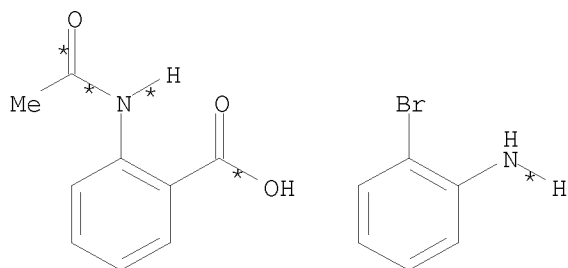
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AT  
YIELD 73%

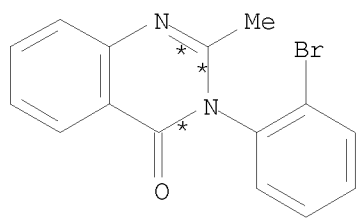
RX(36)      RCT    BJ 89-52-1, BQ 108-42-9  
             RGT    BL 7719-12-2 PC13  
             PRO    AT 340-94-3  
             SOL    108-88-3 PhMe

RX(37) OF 73      BJ    +    BR    ==>    AV...



BJ

BR

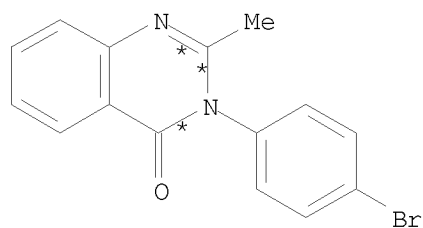
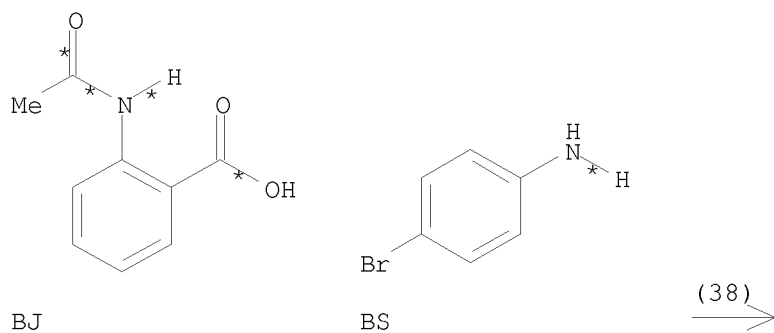


AV  
YIELD 29%

RX(37)      RCT    BJ 89-52-1, BR 615-36-1  
             RGT    BL 7719-12-2 PC13  
             PRO    AV 4260-20-2  
             SOL    108-88-3 PhMe

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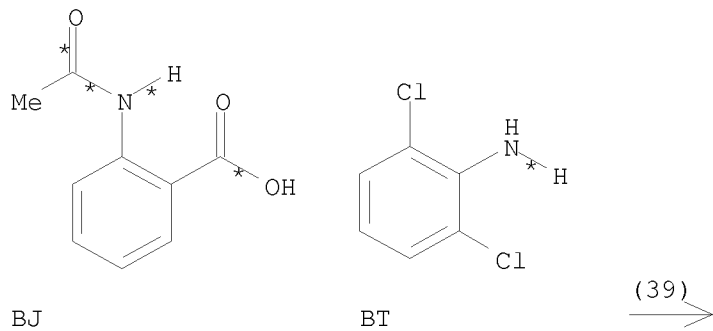
RX(38) OF 73      BJ + BS ==> AX...



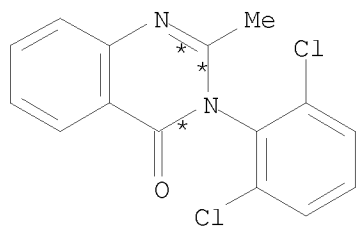
AX  
YIELD 88%

RX(38)      RCT    BJ 89-52-1, BS 106-40-1  
              RGT    BL 7719-12-2 PC13  
              PRO    AX 1788-95-0  
              SOL    108-88-3 PhMe

RX(39) OF 73      BJ + BT ==> BB...



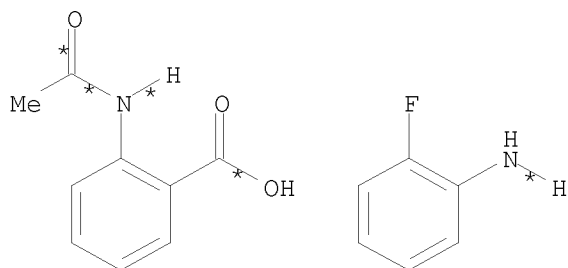
10/ 562,112



BB  
YIELD 33%

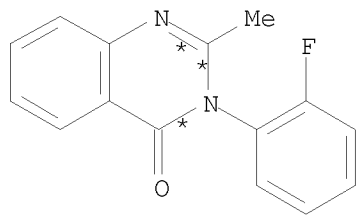
RX(39)      RCT    BJ 89-52-1, BT 608-31-1  
              RGT    BL 7719-12-2 PC13  
              PRO    BB 25509-06-2  
              SOL    108-88-3 PhMe

RX(40) OF 73      BJ    +    BU    ==>    BD...



BJ

BU

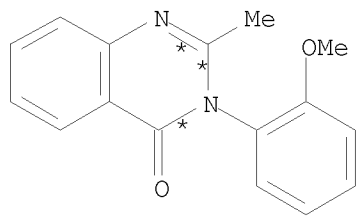
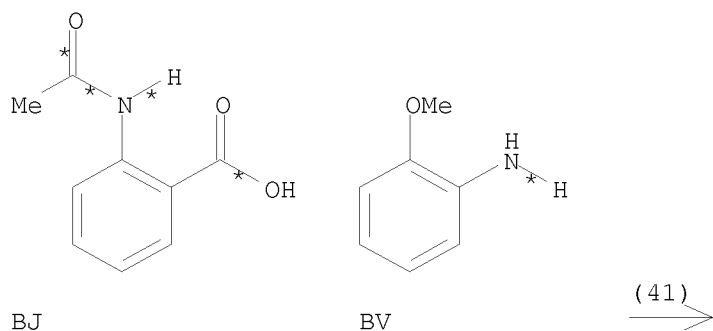


BD  
YIELD 71%

RX(40)      RCT    BJ 89-52-1, BU 348-54-9  
              RGT    BL 7719-12-2 PC13  
              PRO    BD 1897-87-6  
              SOL    108-88-3 PhMe

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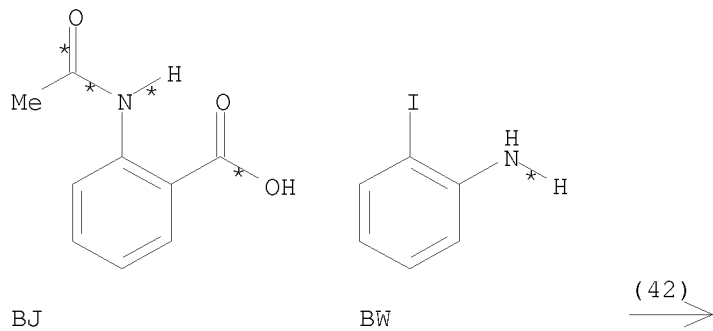
RX(41) OF 73      BJ + BV ==> BF...



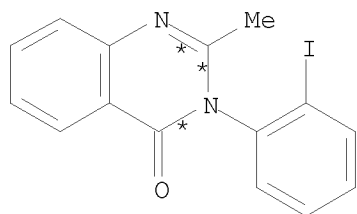
BF  
YIELD 71%

RX(41)      RCT    BJ 89-52-1, BV 90-04-0  
             RGT    BL 7719-12-2 PC13  
             PRO    BF 4260-28-0  
             SOL    108-88-3 PhMe

RX(42) OF 73      BJ + BW ==> BH...



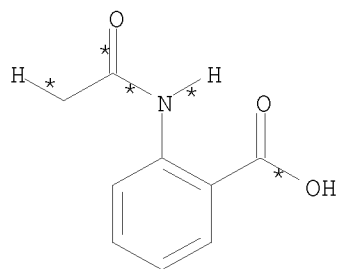
10/ 562,112



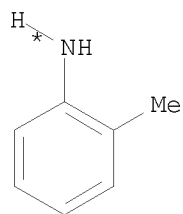
BH  
YIELD 47%

RX(42)      RCT   BJ 89-52-1, BW 615-43-0  
              RGT   BL 7719-12-2 PC13  
              PRO   BH 35289-03-3  
              SOL   108-88-3 PhMe

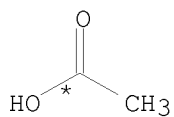
RX(43) OF 73 COMPOSED OF RX(32), RX(1)  
RX(43)      BJ + BK + B ==> C



BJ

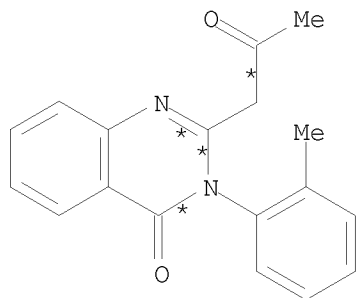


BK



B  
esters

2  
STEPS  
→



C  
YIELD 61%

RX(32)      RCT   BJ 89-52-1, BK 95-53-4  
              RGT   BL 7719-12-2 PC13

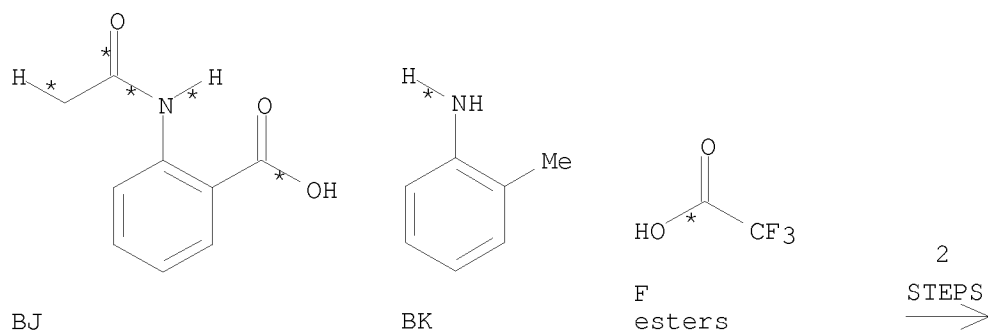


10/ 562,112

PRO A 72-44-6  
SOL 108-88-3 PhMe

RX(1) RCT A 72-44-6, B 64-19-7D  
RGT D 7646-69-7 NaH  
PRO C 73283-07-5  
SOL 110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

RX(44) OF 73 COMPOSED OF RX(32), RX(2)  
RX(44) BJ + BK + F ==> G



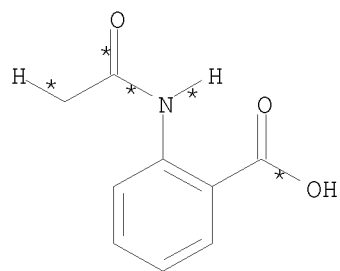
G  
YIELD 87%

RX(32) RCT BJ 89-52-1, BK 95-53-4  
RGT BL 7719-12-2 PC13  
PRO A 72-44-6  
SOL 108-88-3 PhMe

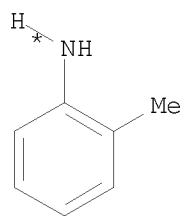
RX(2) RCT A 72-44-6, F 76-05-1D  
RGT D 7646-69-7 NaH  
PRO G 73283-08-6  
SOL 110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

RX(45) OF 73 COMPOSED OF RX(32), RX(3)  
RX(45) BJ + BK + H ==> I

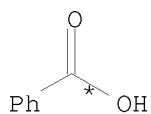
10/ 562,112



BJ

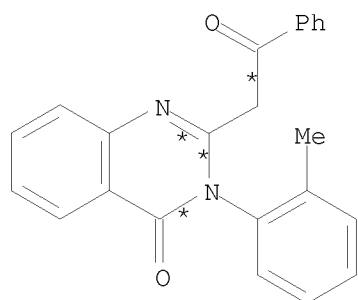


BK



H  
esters

2  
STEPS  
→

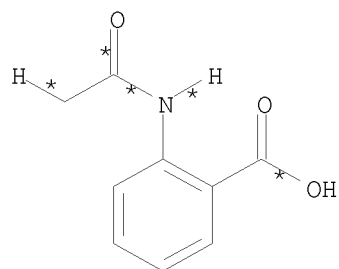


I  
YIELD 80%

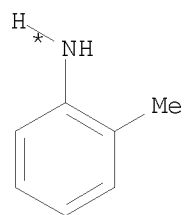
RX(32)     RCT    BJ 89-52-1, BK 95-53-4  
             RGT    BL 7719-12-2 PC13  
             PRO    A 72-44-6  
             SOL    108-88-3 PhMe

RX(3)     RCT    A 72-44-6, H 65-85-0D  
             RGT    D 7646-69-7 NaH  
             PRO    I 73283-14-4  
             SOL    110-71-4 (CH2OMe)2

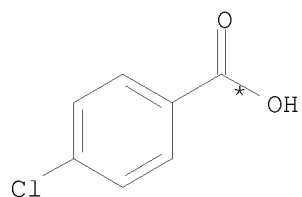
RX(46) OF 73 COMPOSED OF RX(32), RX(4)  
RX(46)     BJ   +   BK   +   J   ==>   K



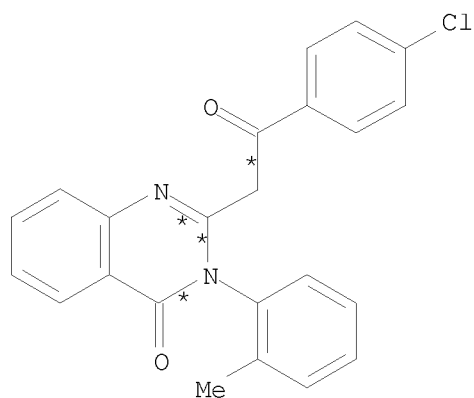
BJ



BK

J  
esters

2  
STEPS  
→

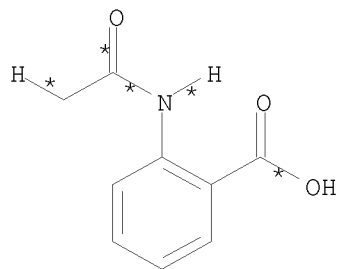
K  
YIELD 74%

RX(32) RCT BJ 89-52-1, BK 95-53-4  
RGT BL 7719-12-2 PC13  
PRO A 72-44-6  
SOL 108-88-3 PhMe

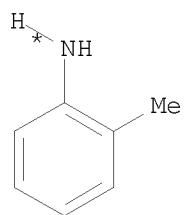
RX(4) RCT A 72-44-6, J 74-11-3D  
RGT D 7646-69-7 NaH  
PRO K 73283-15-5  
SOL 110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

RX(47) OF 73 COMPOSED OF RX(32), RX(5)  
RX(47) BJ + BK + L ==> M

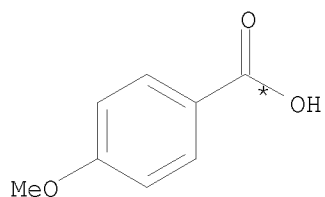
10/ 562,112



BJ

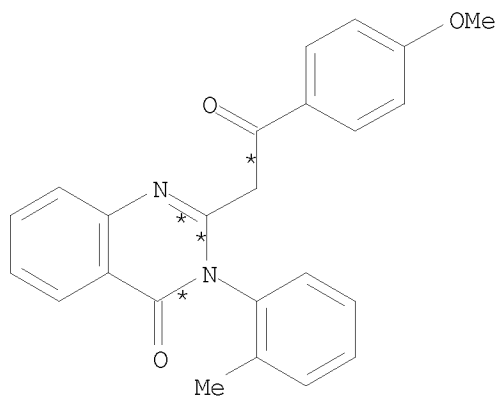


BK



L  
esters

2  
STEPS  
→



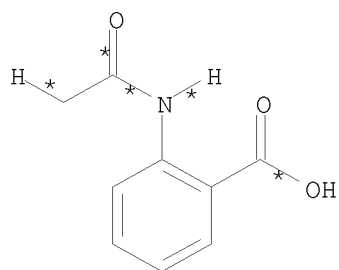
M  
YIELD 72%

RX(32)     RCT   BJ 89-52-1, BK 95-53-4  
           RGT   BL 7719-12-2 PC13  
           PRO   A 72-44-6  
           SOL   108-88-3 PhMe

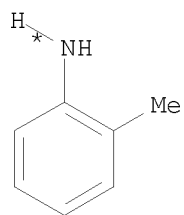
RX(5)     RCT   A 72-44-6, L 100-09-4D  
           RGT   D 7646-69-7 NaH  
           PRO   M 73283-16-6  
           SOL   110-71-4 (CH2OMe)2

RX(48) OF 73 COMPOSED OF RX(32), RX(6)  
RX(48)     BJ   +   BK   +   N   ==>   O

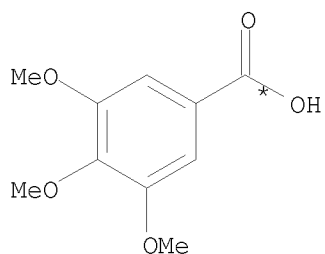
10/ 562,112



BJ

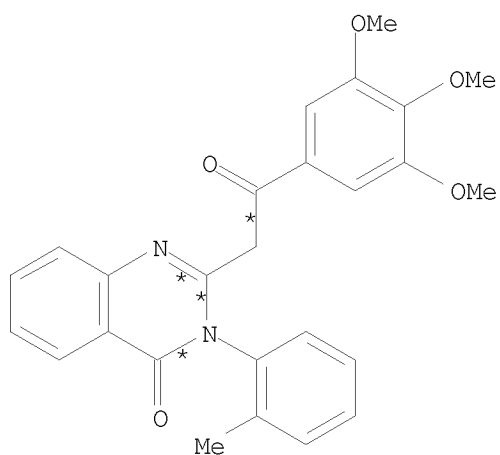


BK



N  
esters

2  
STEPS  
→



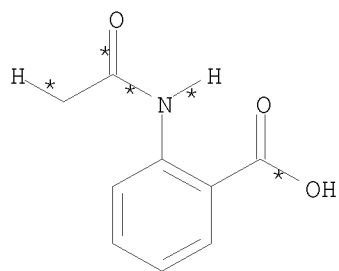
O  
YIELD 67%

RX(32)    RCT    BJ 89-52-1, BK 95-53-4  
           RGT    BL 7719-12-2 PC13  
           PRO    A 72-44-6  
           SOL    108-88-3 PhMe

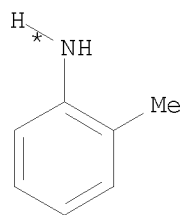
RX(6)     RCT    A 72-44-6, N 118-41-2D  
           RGT    D 7646-69-7 NaH  
           PRO    O 73283-17-7  
           SOL    110-71-4 (CH2OMe)2

RX(49) OF 73 COMPOSED OF RX(32), RX(7)  
 RX(49)    BJ + BK + P ==> Q

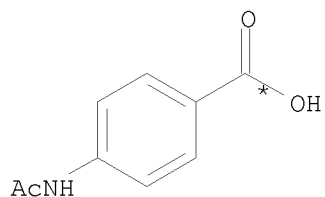
10/ 562,112



BJ

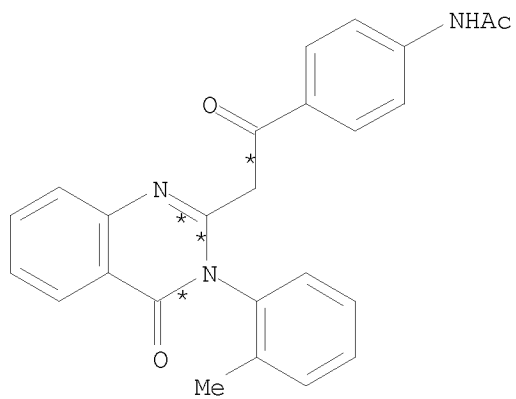


BK



P  
esters

2  
STEPS  
→



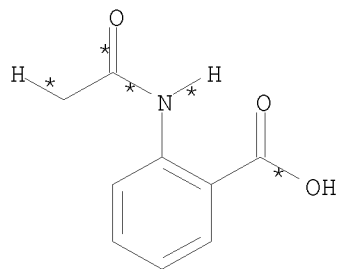
Q  
YIELD 42%

RX(32)     RCT   BJ 89-52-1, BK 95-53-4  
            RGT   BL 7719-12-2 PC13  
            PRO   A 72-44-6  
            SOL   108-88-3 PhMe

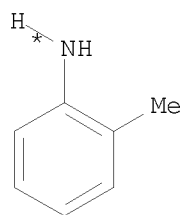
RX(7)      RCT   A 72-44-6, P 556-08-1D  
            RGT   D 7646-69-7 NaH  
            PRO   Q 73283-19-9  
            SOL   109-99-9 THF

RX(50) OF 73 COMPOSED OF RX(32), RX(8)  
RX(50)     BJ   +   BK   +   S   ==>   T

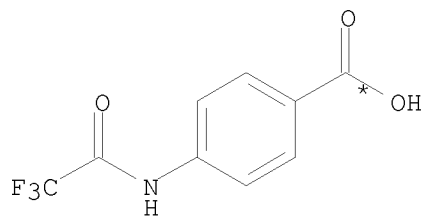
10/ 562,112



BJ

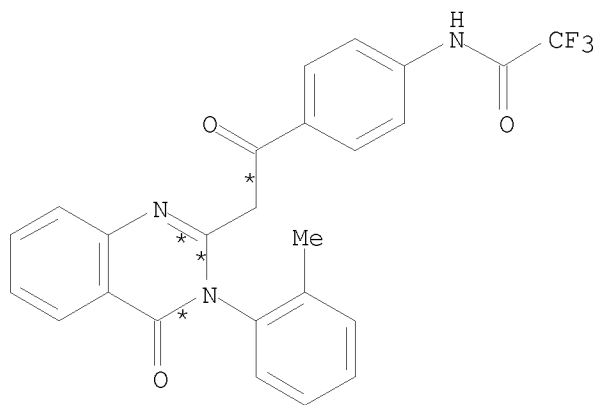


BK



S  
esters

2  
STEPS  
→



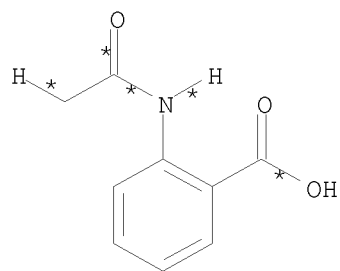
T  
YIELD 47%

RX(32)     RCT   BJ 89-52-1, BK 95-53-4  
           RGT   BL 7719-12-2 PC13  
           PRO   A 72-44-6  
           SOL   108-88-3 PhMe

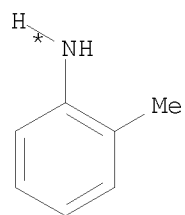
RX(8)     RCT   A 72-44-6, S 404-26-2D  
           RGT   D 7646-69-7 NaH  
           PRO   T 73283-18-8  
           SOL   109-99-9 THF

RX(51) OF 73 COMPOSED OF RX(32), RX(9)  
RX(51)     BJ   +   BK   +   U   ==>   V

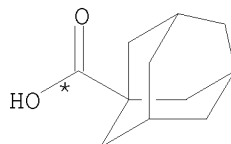
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BJ

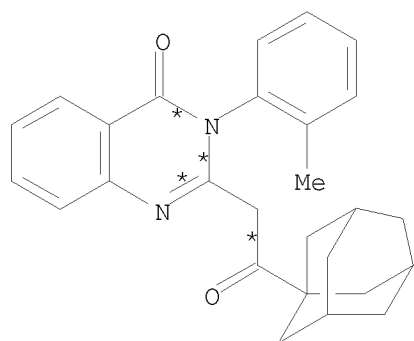


BK



U  
esters

2  
STEPS  
→



V  
YIELD 81%

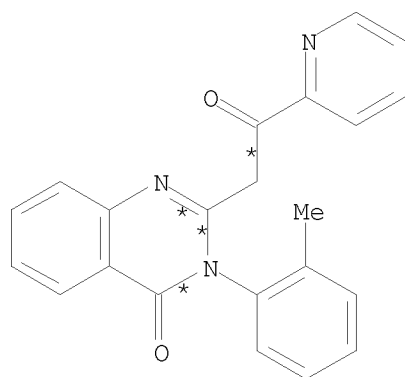
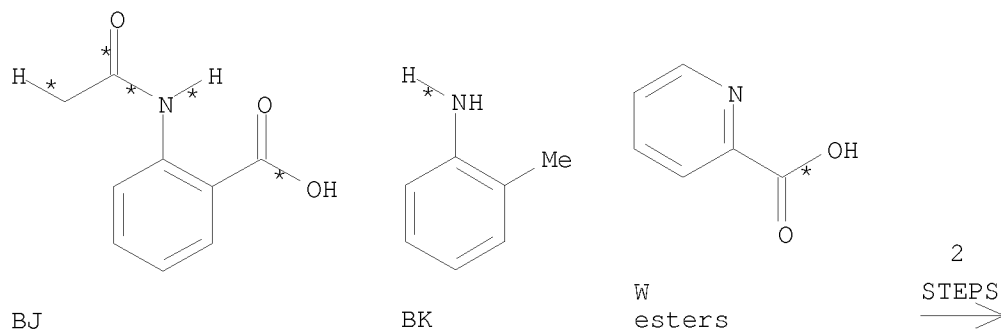
RX(32)     RCT   BJ 89-52-1, BK 95-53-4  
             RGT   BL 7719-12-2 PC13  
             PRO   A 72-44-6  
             SOL   108-88-3 PhMe

RX(9)       RCT   A 72-44-6, U 828-51-3D  
             RGT   D 7646-69-7 NaH  
             PRO   V 73283-12-2  
             SOL   110-71-4 (CH2OMe)2

RX(52) OF 73 COMPOSED OF RX(32), RX(10)  
RX(52)     BJ   +   BK   +   W   ==>   X



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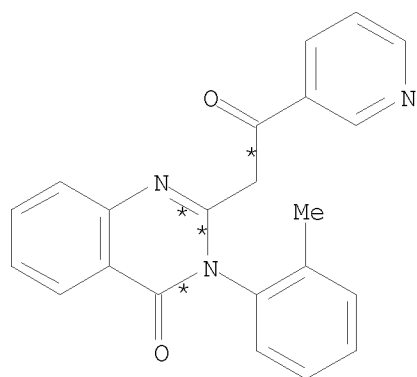
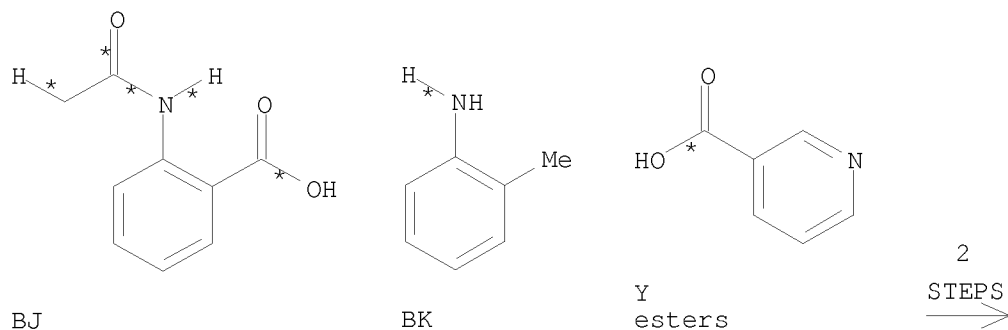
X  
YIELD 80%

RX(32)      RCT    BJ 89-52-1, BK 95-53-4  
              RGT    BL 7719-12-2 PC13  
              PRO    A 72-44-6  
              SOL    108-88-3 PhMe

RX(10)      RCT    A 72-44-6, W 98-98-6D  
              RGT    D 7646-69-7 NaH  
              PRO    X 73283-09-7  
              SOL    110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

RX(53) OF 73 COMPOSED OF RX(32), RX(11)  
RX(53)      BJ + BK + Y ==> Z

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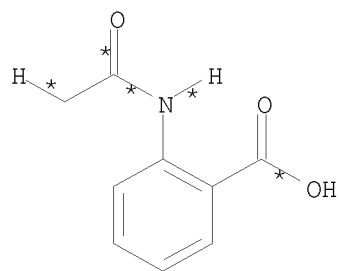
Z  
YIELD 70%

RX(32) RCT BJ 89-52-1, BK 95-53-4  
RGT BL 7719-12-2 PC13  
PRO A 72-44-6  
SOL 108-88-3 PhMe

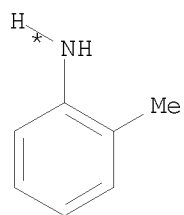
RX(11) RCT A 72-44-6, Y 59-67-6D  
RGT D 7646-69-7 NaH  
PRO Z 73283-10-0  
SOL 110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

RX(54) OF 73 COMPOSED OF RX(32), RX(12)  
RX(54) BJ + BK + AA ==> AB

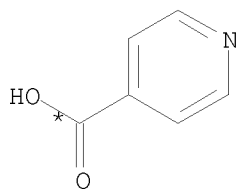
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BJ

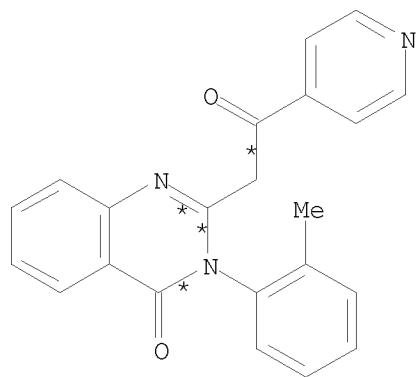


BK



AA  
esters

2  
STEPS  
→



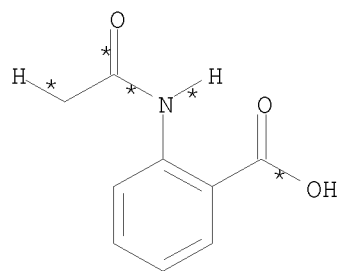
AB  
YIELD 85%

RX(32)     RCT    BJ 89-52-1, BK 95-53-4  
             RGT    BL 7719-12-2 PC13  
             PRO    A 72-44-6  
             SOL    108-88-3 PhMe

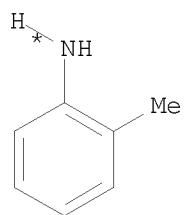
RX(12)     RCT    A 72-44-6, AA 55-22-1D  
             RGT    D 7646-69-7 NaH  
             PRO    AB 73283-11-1  
             SOL    110-71-4 (CH2OMe)2

RX(55) OF 73 COMPOSED OF RX(32), RX(13)  
RX(55)     BJ + BK + AC ==> AD

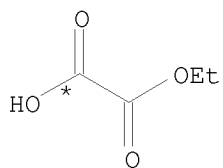
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BJ

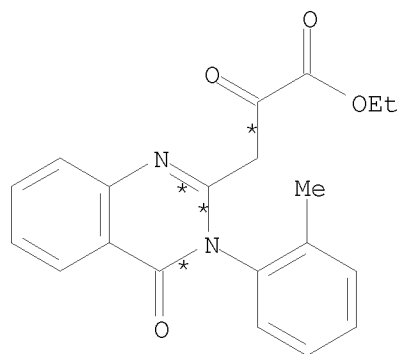


BK



AC  
esters

2  
STEPS  
→



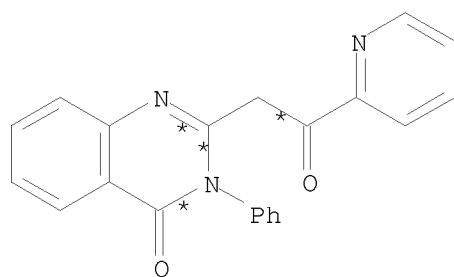
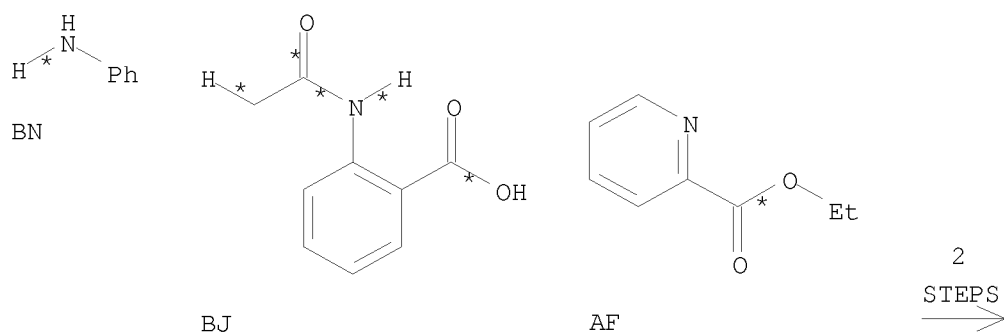
AD  
YIELD 62%

RX(32)     RCT    BJ 89-52-1, BK 95-53-4  
             RGT    BL 7719-12-2 PC13  
             PRO    A 72-44-6  
             SOL    108-88-3 PhMe

RX(13)     RCT    A 72-44-6, AC 617-37-8D  
             RGT    D 7646-69-7 NaH  
             PRO    AD 56232-60-1  
             SOL    110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

RX(56) OF 73 COMPOSED OF RX(33), RX(14)  
RX(56)     BN + BJ + AF ==> AG

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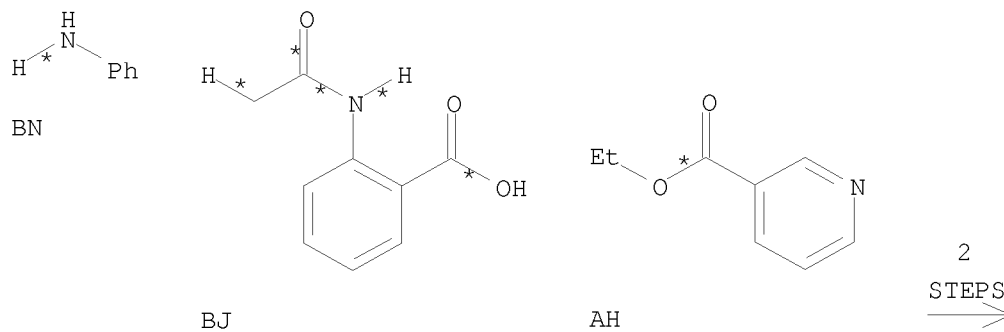


AG  
YIELD 76%

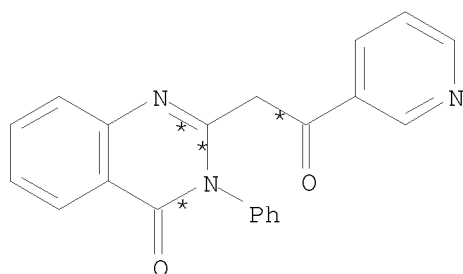
RX(33) RCT BN 62-53-3, BJ 89-52-1  
RGT BL 7719-12-2 PC13  
PRO AE 2385-23-1  
SOL 108-88-3 PhMe

RX(14) RCT AE 2385-23-1, AF 2524-52-9  
RGT D 7646-69-7 NaH  
PRO AG 73283-25-7  
SOL 110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

RX(57) OF 73 COMPOSED OF RX(33), RX(15)  
RX(57) BN + BJ + AH ==> AI



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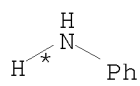


AI  
YIELD 72%

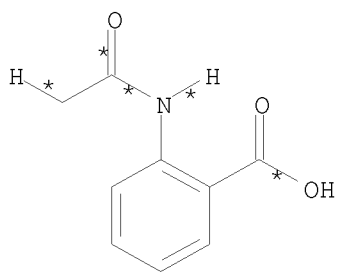
RX(33)      RCT    BN 62-53-3, BJ 89-52-1  
              RGT    BL 7719-12-2 PC13  
              PRO    AE 2385-23-1  
              SOL    108-88-3 PhMe

RX(15)      RCT    AE 2385-23-1, AH 614-18-6  
              RGT    D 7646-69-7 NaH  
              PRO    AI 73283-26-8  
              SOL    110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

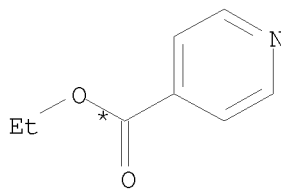
RX(58) OF 73 COMPOSED OF RX(33), RX(16)  
RX(58)      BN + BJ + AJ ==> AK



BN



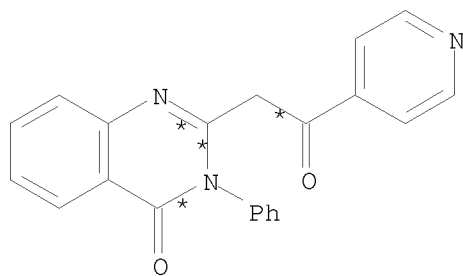
BJ



AJ

2  
STEPS  
→

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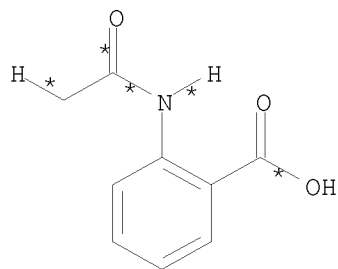


AK  
YIELD 62%

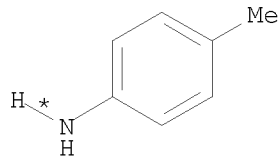
RX(33)      RCT    BN 62-53-3, BJ 89-52-1  
              RGT    BL 7719-12-2 PC13  
              PRO    AE 2385-23-1  
              SOL    108-88-3 PhMe

RX(16)      RCT    AE 2385-23-1, AJ 1570-45-2  
              RGT    D 7646-69-7 NaH  
              PRO    AK 73283-27-9  
              SOL    110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

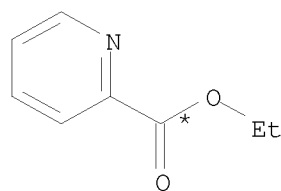
RX(59) OF 73 COMPOSED OF RX(34), RX(17)  
RX(59)      BJ    +    BO    +    AF    ==>    AM



BJ



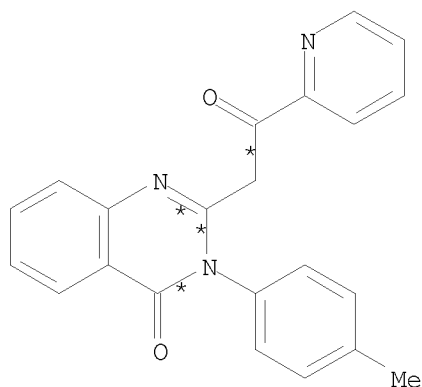
BO



AF

2  
STEPS  
→

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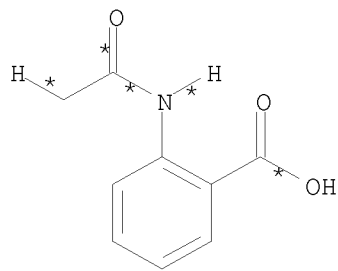
AM

YIELD 76%

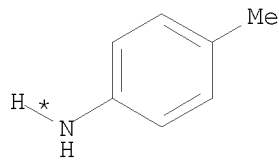
RX(34)      RCT    BJ 89-52-1, BO 106-49-0  
              RGT    BL 7719-12-2 PC13  
              PRO    AL 22316-59-2  
              SOL    108-88-3 PhMe

RX(17)      RCT    AL 22316-59-2, AF 2524-52-9  
              RGT    D 7646-69-7 NaH  
              PRO    AM 73283-29-1  
              SOL    110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

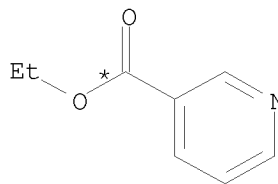
RX(60) OF 73 COMPOSED OF RX(34), RX(18)  
RX(60)      BJ + BO + AH ==> AN



BJ



BO

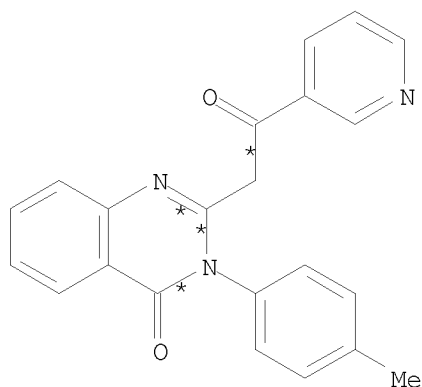


AH

2  
STEPS  
→



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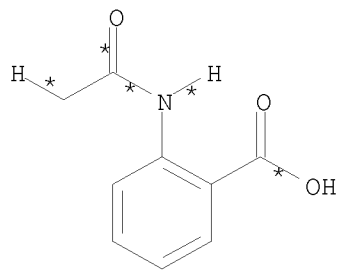


AN  
YIELD 81%

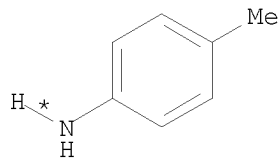
RX(34)      RCT    BJ 89-52-1, BO 106-49-0  
              RGT    BL 7719-12-2 PC13  
              PRO    AL 22316-59-2  
              SOL    108-88-3 PhMe

RX(18)      RCT    AL 22316-59-2, AH 614-18-6  
              RGT    D 7646-69-7 NaH  
              PRO    AN 73283-30-4  
              SOL    110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

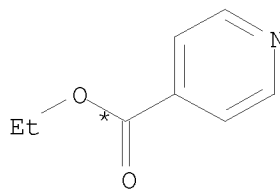
RX(61) OF 73 COMPOSED OF RX(34), RX(19)  
RX(61)      BJ + BO + AJ ==> AO



BJ



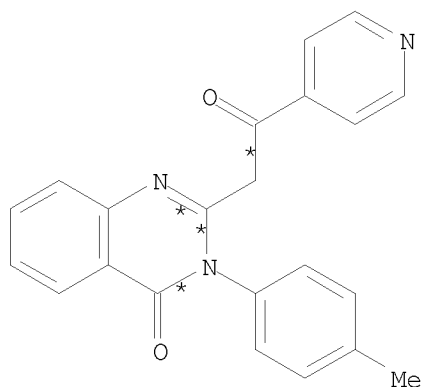
BO



AJ

2  
STEPS  
→

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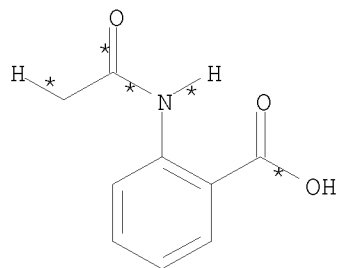
AO

YIELD 84%

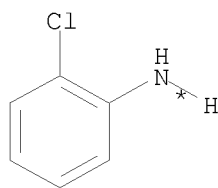
RX(34) RCT BJ 89-52-1, BO 106-49-0  
RGT BL 7719-12-2 PC13  
PRO AL 22316-59-2  
SOL 108-88-3 PhMe

RX(19) RCT AL 22316-59-2, AJ 1570-45-2  
RGT D 7646-69-7 NaH  
PRO AO 73283-31-5  
SOL 110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

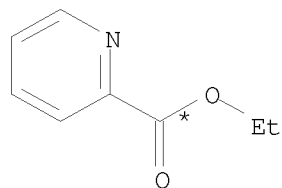
RX(62) OF 73 COMPOSED OF RX(35), RX(20)  
RX(62) BJ + BP + AF ==> AQ



BJ



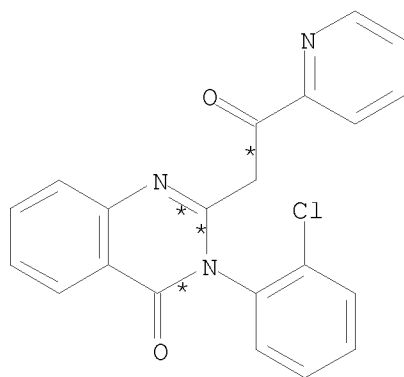
BP



AF

2  
STEPS  
→

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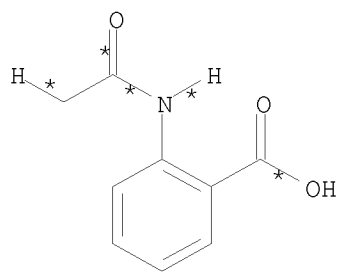


AQ  
YIELD 82%

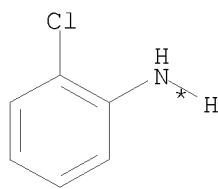
RX(35)      RCT    BJ 89-52-1, BP 95-51-2  
              RGT    BL 7719-12-2 PC13  
              PRO    AP 340-57-8  
              SOL    108-88-3 PhMe

RX(20)      RCT    AP 340-57-8, AF 2524-52-9  
              RGT    D 7646-69-7 NaH  
              PRO    AQ 73283-21-3  
              SOL    110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

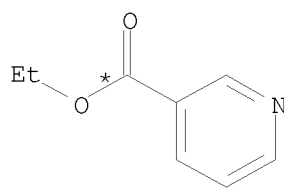
RX(63) OF 73 COMPOSED OF RX(35), RX(21)  
RX(63)      BJ + BP + AH ==> AR



BJ



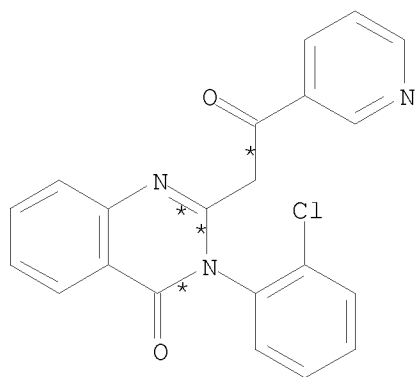
BP



AH

2  
STEPS  
→

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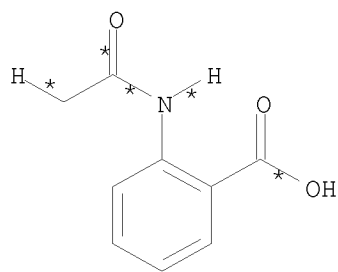


AR  
YIELD 79%

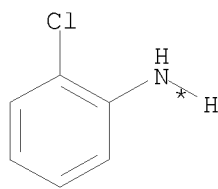
RX(35) RCT BJ 89-52-1, BP 95-51-2  
RGT BL 7719-12-2 PC13  
PRO AP 340-57-8  
SOL 108-88-3 PhMe

RX(21) RCT AP 340-57-8, AH 614-18-6  
RGT D 7646-69-7 NaH  
PRO AR 73283-22-4  
SOL 110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

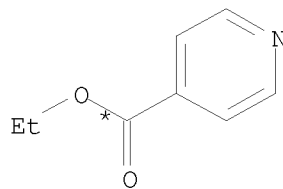
RX(64) OF 73 COMPOSED OF RX(35), RX(22)  
RX(64) BJ + BP + AJ ==> AS



BJ



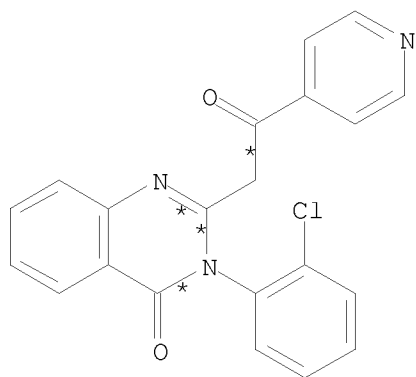
BP



AJ

2  
STEPS  
→

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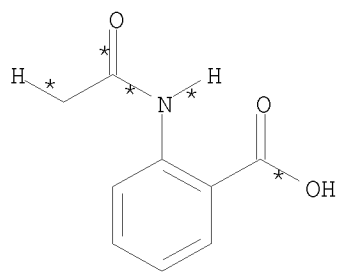


AS  
YIELD 92%

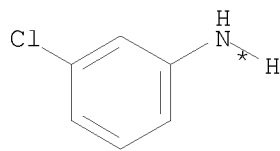
RX(35)      RCT    BJ 89-52-1, BP 95-51-2  
              RGT    BL 7719-12-2 PC13  
              PRO    AP 340-57-8  
              SOL    108-88-3 PhMe

RX(22)      RCT    AP 340-57-8, AJ 1570-45-2  
              RGT    D 7646-69-7 NaH  
              PRO    AS 73283-23-5  
              SOL    110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

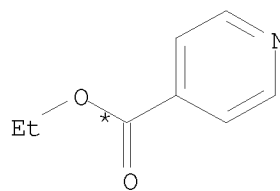
RX(65) OF 73 COMPOSED OF RX(36), RX(23)  
RX(65)      BJ + BQ + AJ ==> AU



BJ



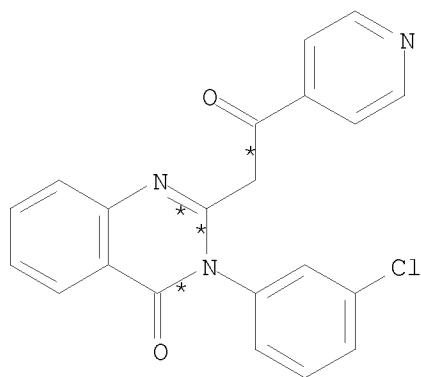
BQ



AJ

2  
STEPS  
→

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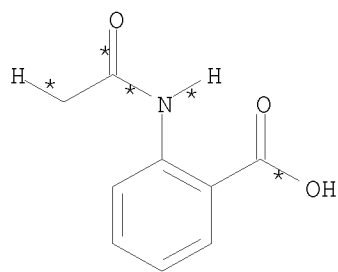


AU  
YIELD 70%

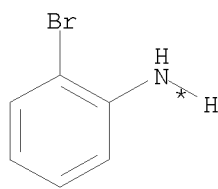
RX(36)      RCT    BJ 89-52-1, BQ 108-42-9  
              RGT    BL 7719-12-2 PC13  
              PRO    AT 340-94-3  
              SOL    108-88-3 PhMe

RX(23)      RCT    AT 340-94-3, AJ 1570-45-2  
              RGT    D 7646-69-7 NaH  
              PRO    AU 123382-21-8  
              SOL    110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

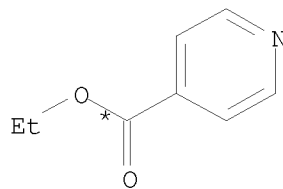
RX(66) OF 73 COMPOSED OF RX(37), RX(24)  
RX(66)      BJ + BR + AJ ==> AW



BJ



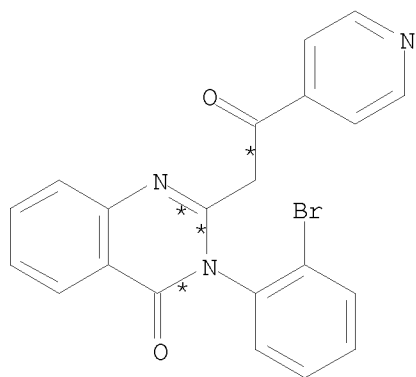
BR



AJ

2  
STEPS  
→

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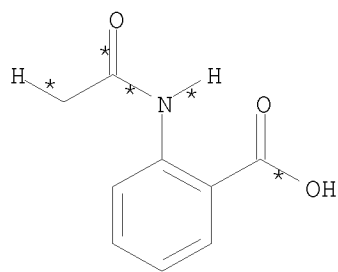


AW  
YIELD 70%

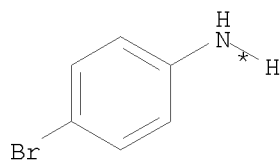
RX(37) RCT BJ 89-52-1, BR 615-36-1  
RGT BL 7719-12-2 PC13  
PRO AV 4260-20-2  
SOL 108-88-3 PhMe

RX(24) RCT AV 4260-20-2, AJ 1570-45-2  
RGT D 7646-69-7 NaH  
PRO AW 123382-22-9  
SOL 110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

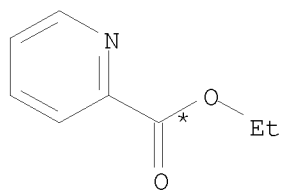
RX(67) OF 73 COMPOSED OF RX(38), RX(25)  
RX(67) BJ + BS + AF ==> AY



BJ



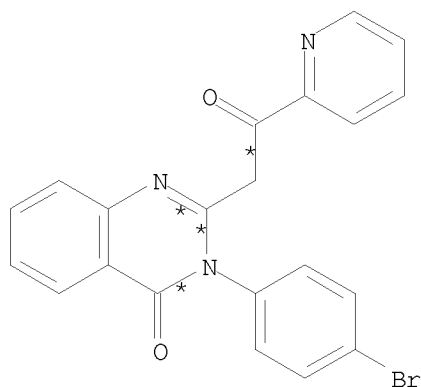
BS



AF

2  
STEPS  
→

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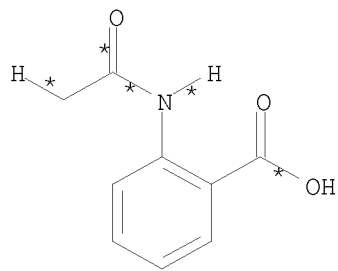


AY  
YIELD 96%

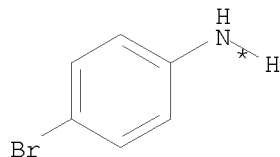
RX(38)      RCT    BJ 89-52-1, BS 106-40-1  
              RGT    BL 7719-12-2 PC13  
              PRO    AX 1788-95-0  
              SOL    108-88-3 PhMe

RX(25)      RCT    AX 1788-95-0, AF 2524-52-9  
              RGT    D 7646-69-7 NaH  
              PRO    AY 73283-33-7  
              SOL    110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

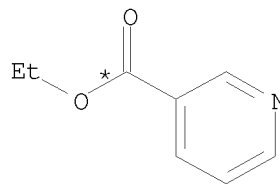
RX(68) OF 73 COMPOSED OF RX(38), RX(26)  
RX(68)      BJ + BS + AH ==> AZ



BJ



BS

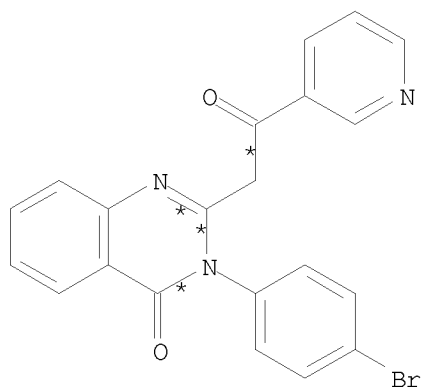


AH

2  
STEPS  
→



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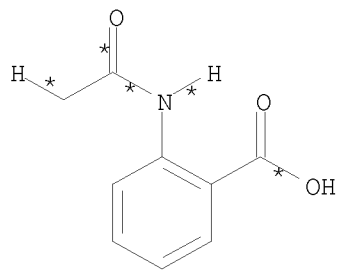


AZ  
YIELD 92%

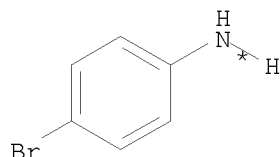
RX(38)     RCT    BJ 89-52-1, BS 106-40-1  
             RGT    BL 7719-12-2 PC13  
             PRO    AX 1788-95-0  
             SOL    108-88-3 PhMe

RX(26)     RCT    AX 1788-95-0, AH 614-18-6  
             RGT    D 7646-69-7 NaH  
             PRO    AZ 73283-34-8  
             SOL    110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

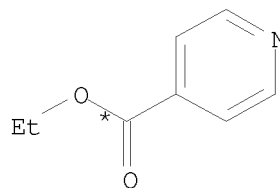
RX(69) OF 73 COMPOSED OF RX(38), RX(27)  
RX(69)     BJ + BS + AJ ==> BA



BJ



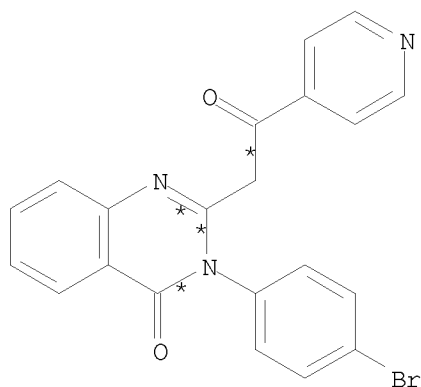
BS



AJ

2  
STEPS  
→

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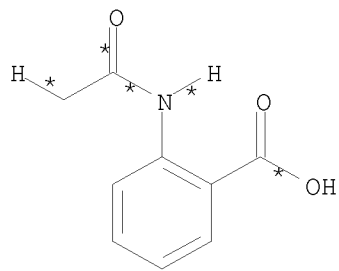


BA  
YIELD 90%

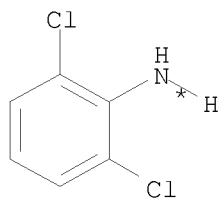
RX(38)      RCT    BJ 89-52-1, BS 106-40-1  
              RGT    BL 7719-12-2 PC13  
              PRO    AX 1788-95-0  
              SOL    108-88-3 PhMe

RX(27)      RCT    AX 1788-95-0, AJ 1570-45-2  
              RGT    D 7646-69-7 NaH  
              PRO    BA 73283-35-9  
              SOL    110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

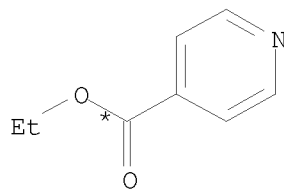
RX(70) OF 73 COMPOSED OF RX(39), RX(28)  
RX(70)      BJ + BT + AJ ==> BC



BJ



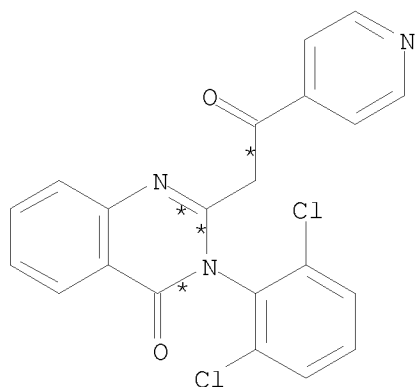
BT



AJ

2  
STEPS  
→

10/ 562,112

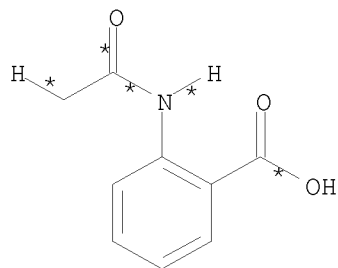


BC  
YIELD 72%

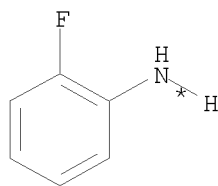
RX(39)      RCT    BJ 89-52-1, BT 608-31-1  
              RGT    BL 7719-12-2 PC13  
              PRO    BB 25509-06-2  
              SOL    108-88-3 PhMe

RX(28)      RCT    BB 25509-06-2, AJ 1570-45-2  
              RGT    D 7646-69-7 NaH  
              PRO    BC 123382-23-0  
              SOL    110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

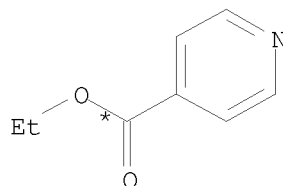
RX(71) OF 73 COMPOSED OF RX(40), RX(29)  
RX(71)      BJ + BU + AJ ==> BE



BJ



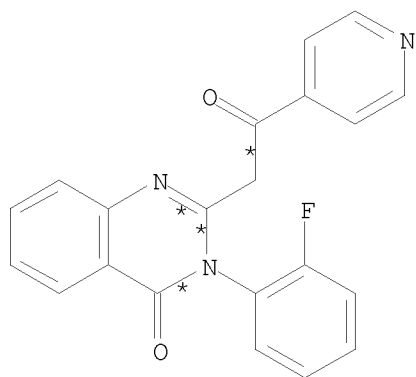
BU



AJ

2  
STEPS  
→

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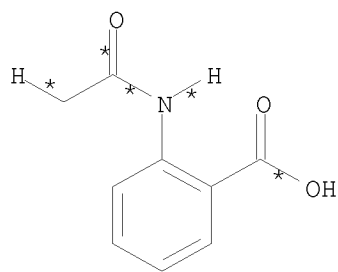


BE  
YIELD 69%

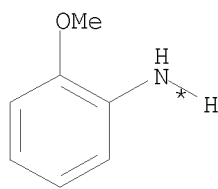
RX(40)      RCT    BJ 89-52-1, BU 348-54-9  
              RGT    BL 7719-12-2 PC13  
              PRO    BD 1897-87-6  
              SOL    108-88-3 PhMe

RX(29)      RCT    BD 1897-87-6, AJ 1570-45-2  
              RGT    D 7646-69-7 NaH  
              PRO    BE 123382-24-1  
              SOL    110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

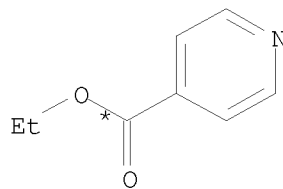
RX(72) OF 73 COMPOSED OF RX(41), RX(30)  
RX(72)      BJ + BV + AJ ==> BG



BJ



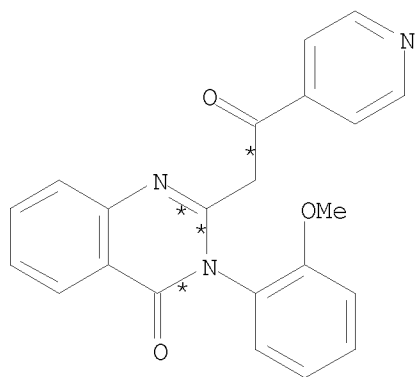
BV



AJ

2  
STEPS  
→

10/ 562,112

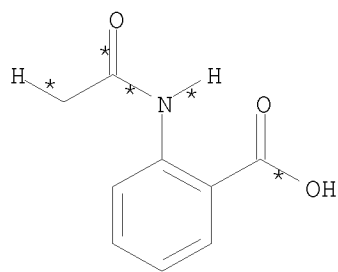


BG  
YIELD 70%

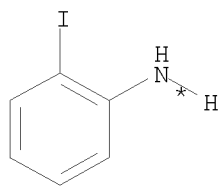
RX(41) RCT BJ 89-52-1, BV 90-04-0  
RGT BL 7719-12-2 PC13  
PRO BF 4260-28-0  
SOL 108-88-3 PhMe

RX(30) RCT BF 4260-28-0, AJ 1570-45-2  
RGT D 7646-69-7 NaH  
PRO BG 123382-25-2  
SOL 110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

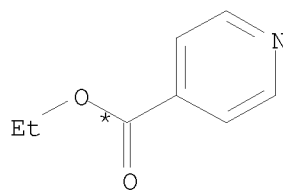
RX(73) OF 73 COMPOSED OF RX(42), RX(31)  
RX(73) BJ + BW + AJ ==> BI



BJ



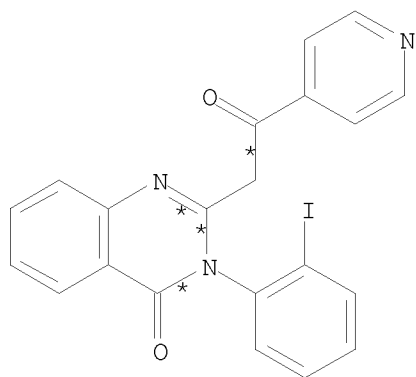
BW



AJ

2  
STEPS  
→

10/ 562,112

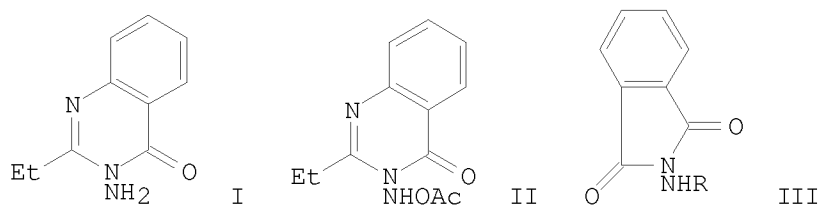


BI  
YIELD 46%

RX(42) RCT BJ 89-52-1, BW 615-43-0  
RGT BL 7719-12-2 PC13  
PRO BH 35289-03-3  
SOL 108-88-3 PhMe

RX(31) RCT BH 35289-03-3, AJ 1570-45-2  
RGT D 7646-69-7 NaH  
PRO BI 123382-26-3  
SOL 110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>

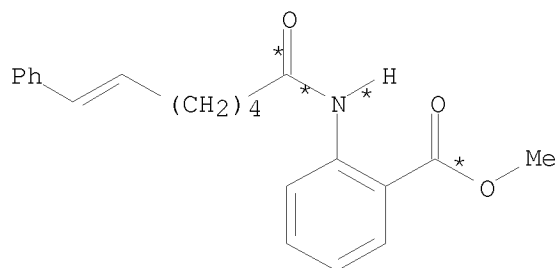
L3 ANSWER 161 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 112:35789 CASREACT  
TITLE: Aziridination by oxidative addition of  
N-aminoquinazolones to alkenes: evidence for  
non-involvement of N-nitrenes  
AUTHOR(S): Atkinson, Robert S.; Grimshire, Michael J.; Kelly,  
Brian J.  
CORPORATE SOURCE: Dep. Chem., Leicester Univ., Leicester, LE1 7RH, UK  
SOURCE: Tetrahedron (1989), 45(10), 2875-86  
CODEN: TETRAB; ISSN: 0040-4020  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



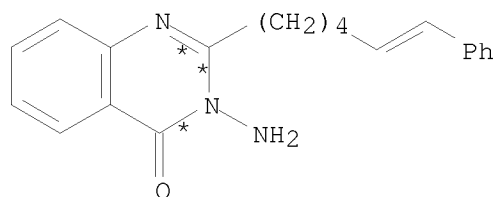
AB Oxidation of 3-aminoquinazolones, e.g., I, with Pb(OAc)<sub>4</sub> at -20° gives

N-(acetoxiamino)quinazolones, e.g., II, which are stable in solution at this temperature. The latter compds. function as inter- and intramol. aziridinating agents for alkenes and appear to play the role previously ascribed to the corresponding N-nitrenes. An analogous N-acetoxiaminophthalimide intermediate III (R = OAc) is implicated in the Pb(OAc)<sub>4</sub> oxidation of III (R = H).

RX(16) OF 19 AJ ==> V...



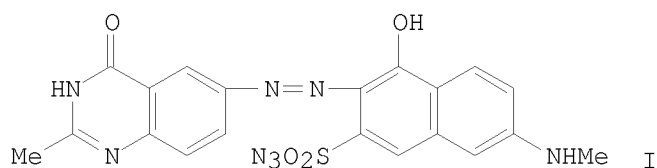
AJ



V

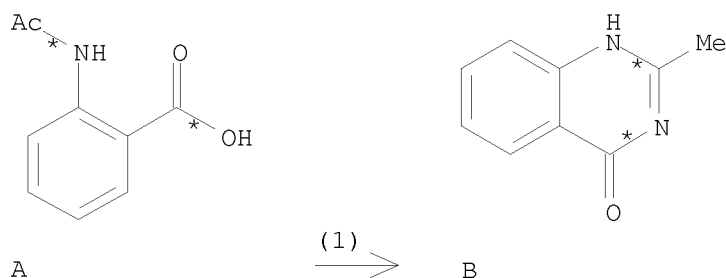
RX(16) RCT AJ 124553-59-9  
 RGT AK 302-01-2 N2H4  
 PRO V 124553-47-5  
 SOL 64-17-5 EtOH

L3 ANSWER 162 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 112:8700 CASREACT  
 TITLE: Reactive disperse dyes. Synthesis of sulfonylazido group reactive disperse dyes and their application on nylon and polyester fibers  
 AUTHOR(S): Naik, N. M.; Desai, K. R.  
 CORPORATE SOURCE: Dep. Chem., South Gujarat Univ., Surat, 395 007, India  
 SOURCE: Journal of the Indian Chemical Society (1989), 66(7), 495-7  
 CODEN: JICSAH; ISSN: 0019-4522  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



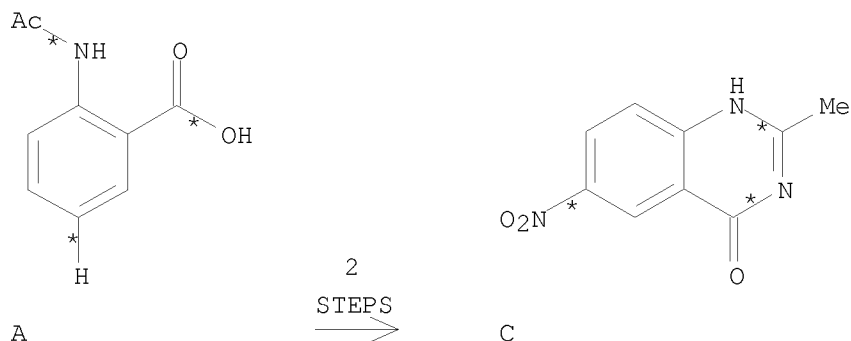
AB 2-Methyl-6-amino-4-quinazolinone was diazotized and coupled with sulfo group-containing hydroxynaphthalenes or pyrazolones and the sulfo group of the product was converted to the sulfonyl azide via the chloride. For example, I was obtained from N-Me J acid. The sulfonyl azides prepared (8) were used as reactive disperse dyes on polyamide and polyester fiber.

RX(1) OF 10 A ==> B...



RX(1) RCT A 89-52-1  
PRO B 1769-24-0

RX(5) OF 10 COMPOSED OF RX(1), RX(2)  
RX(5) A ==> C

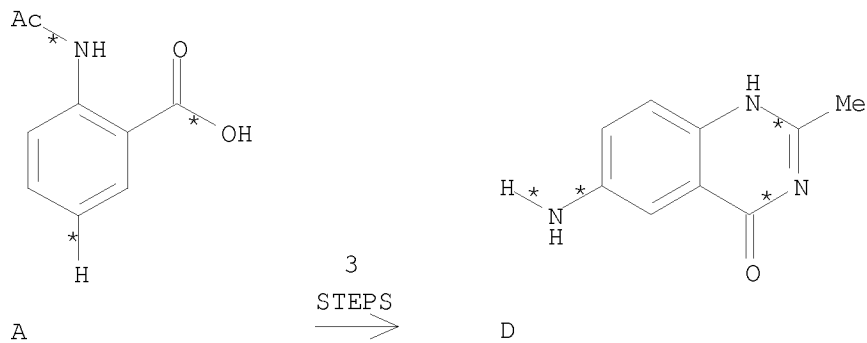


RX(1) RCT A 89-52-1  
PRO B 1769-24-0

RX(2) RCT B 1769-24-0  
PRO C 24688-36-6



RX(8) OF 10 COMPOSED OF RX(1), RX(2), RX(3)  
RX(8)            A    ==> D



RX (1)	RCT	A	89-52-1
	PRO	B	1769-24-0

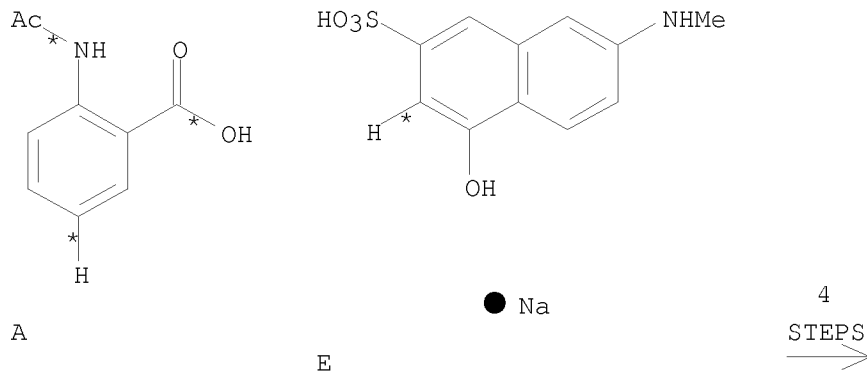
RX (2)	RCT	B	1769-24-0
	PRO	C	24688-36-6

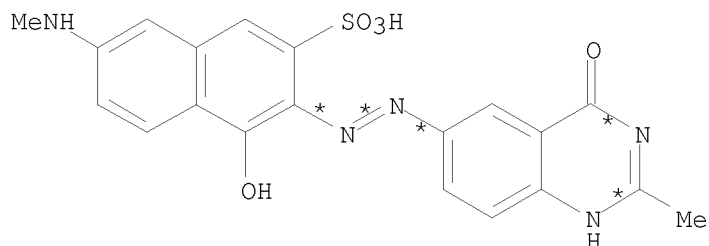
RX (3)	RCT	C	24688-36-6
	PRO	D	17329-24-7

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RX(10) OF 10 COMPOSED OF RX(1), RX(2), RX(3), RX(4)
RX(10)      A  +  E  ==>  F

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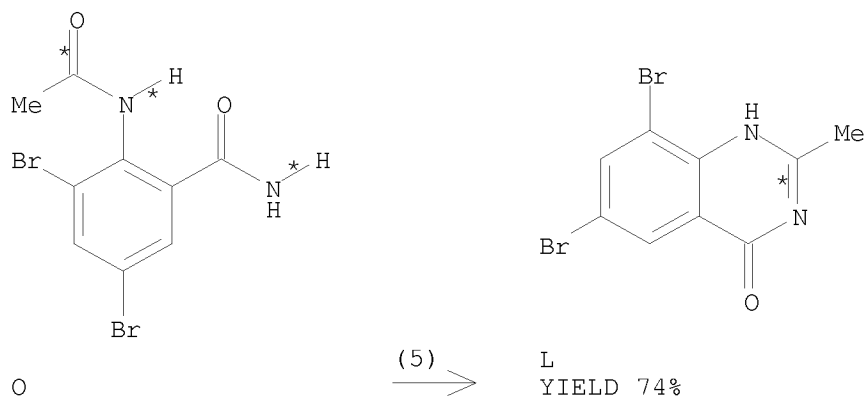
● Na

F

RX(1)	RCT	A	89-52-1
	PRO	B	1769-24-0
RX(2)	RCT	B	1769-24-0
	PRO	C	24688-36-6
RX(3)	RCT	C	24688-36-6
	PRO	D	17329-24-7
RX(4)	RCT	D	17329-24-7, E 41494-91-1
	PRO	F	124190-79-0

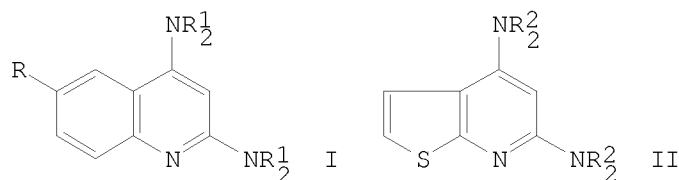
L3 ANSWER 163 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 111:194703 CASREACT  
 TITLE: 6,8-Dibromo-2-methyl-1,3-4(3H)-quinazolinones  
 AUTHOR(S): Ossmann, A. E.; El-Zahabi, M. M.; El-Hakim, A. E.;  
 Osman, A. N.  
 CORPORATE SOURCE: Org. Dep., Fac. Pharm., Cairo, Egypt  
 SOURCE: Pharmazie (1989), 44(2), 113-14  
 CODEN: PHARAT; ISSN: 0031-7144  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Hydrazinolysis of 6,8-dibromo-2-methyl-3,1-benzoxazin-4(H)-one afforded 3-amino-6,8-dibromo-2-methyl-1,3-4(3H)-quinazoline (I). Acylation of the latter with Ac<sub>2</sub>O and BzCl yielded the corresponding acetyl and benzoyl derivs., resp. The diazotization of I with nitrous acid led to reductive deamination and the production of 6,8-dibromo-2-methyl-1,3-4(3H)-quinazolinone.

RX(5) OF 12 ...0 ==&gt; L



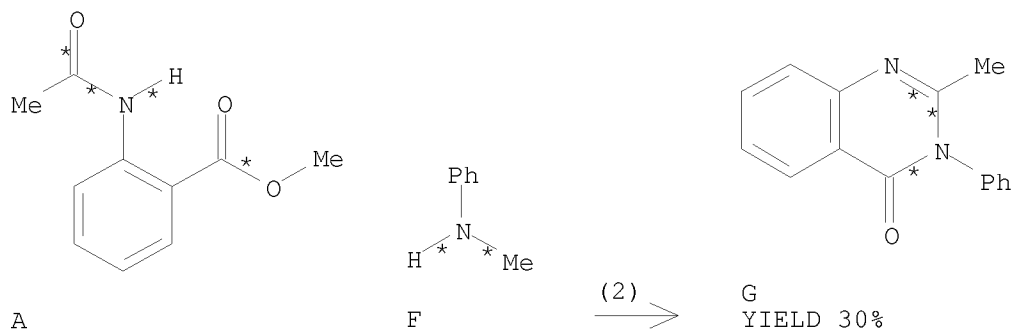
RX(5)      RCT   O 123434-55-9  
              RGT   F 108-24-7 Ac2O  
              PRO   L 82326-77-0

L3      ANSWER 164 OF 258      CASREACT      COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER:      111:153665      CASREACT  
 TITLE:      New one-step synthesis of  
                  2,4-bis(dialkylamino)quinolines and  
                  4,6-bis(dialkylamino)thieno[2,3-b]pyridines  
 AUTHOR(S):      Jensen, Jorgen A.; Pedersen, Erik B.  
 CORPORATE SOURCE:      Dep. Chem., Odense Univ., Odense, DK-5230, Den.  
 SOURCE:      Chemica Scripta (1988), 28(4), 435-7  
                  CODEN: CSRPB9; ISSN: 0004-2056  
 DOCUMENT TYPE:      Journal  
 LANGUAGE:      English  
 GI



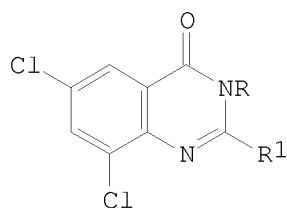
AB      2,4-Bis(dialkylamino)quinolines I (R = H, NR12 = morpholino, Et2N; R = H, Me, NR22 = piperidino, pyrrolidino) were prepared by heating N-acetylanthranilates in a mixture of P2O5, a dialkylamine hydrochloride, and N,N-dimethylcyclohexylamine at 210° for 6-10.5 h. In the same way 4,6-bis(dialkylamino)thieno[2,3-b]pyridines II (NR22 = piperidino, pyrrolidino) were prepared from Me 2-acetamido-3-thiophenecarboxylate.

RX(2) OF 12      A + F ==> G



RX(2) RCT A 2719-08-6, F 100-61-8  
 RGT D 1314-56-3 P2O5, E 98-94-2 C6H11NMe2, H 121-44-8 Et3N  
 PRO G 2385-23-1

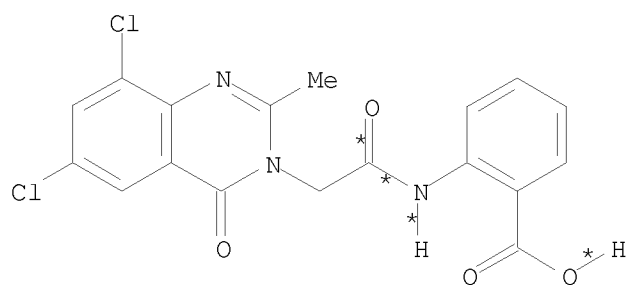
L3 ANSWER 165 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 111:130542 CASREACT  
 TITLE: Synthesis and screening of some newer  
 6,8-dichloro-2-methyl-3-(substituted)-4(3H)-  
 quinazolinones as antimicrobial agents  
 AUTHOR(S): Mohamed, Y. A.; Ammar, Y. A.; El-Sharief, A. M. S.;  
 Ahmed, H.  
 CORPORATE SOURCE: Fac. Sci., Al-Azhar Univ., Nasr, Egypt  
 SOURCE: Proceedings of the Indian National Science Academy,  
 Part A: Physical Sciences (1989), 55(1), 87-95  
 CODEN: PIPSBD; ISSN: 0370-0046  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



- I,  $R = C_6H_4SO_2NHR^2$ ,  $R^1 = Me$   
 II,  $R = NHCOCH_2Cl$ ,  $R^1 = Me$   
 III,  $R = NHCOCH_2NHR^2$ ,  $R^1 = Me$   
 IV,  $R = NH_2$ ,  $R^1 = Me$   
 V,  $R = N=CHAr$ ,  $R^1 = Me$   
 VI,  $R = N=CHAr$ ,  $R^1 = CH=CHAr$   
 VII,  $R = CH_2COCl$ ,  $R^1 = Me$   
 VIII,  $R = CH_2CONHR^2$ ,  $R^1 = Me$   
 IX,  $R = 4\text{-oxo-2H-3,1-benzoxazinylmethyl}$ ,  $R^1 = Me$

AB 6,8-Dichloro-2-methyl-3-(4-N-substituted sulfonamidophenyl)-4(3H)-quinazolinones (I,  $R^2 = H$ , or heterocyclic or  $NHR^2 = \text{guanidino}$ ) were prepared by reaction of 6,8-dichloro-2-methyl-2H-3,1-benzoxazin-4-one with sulfonamides. Also, II was prepared and condensed with amines to give III ( $R^2 = \text{iso-Bu}$ ,  $CH_2Ph$ ,  $C_6H_4OMe-4$ , or sulfonamido group). Condensation of IV with aldehydes under different conditions gave V and VI. VII underwent condensation with amines to give VIII ( $R^2 = \text{aromatic or sulfonamido group}$ ). Cyclization of VIII ( $R^2 = C_6H_4CO_2H-2$ ) with  $Ac_2O$  gave IX. Some of these compds. showed antimicrobial activity.

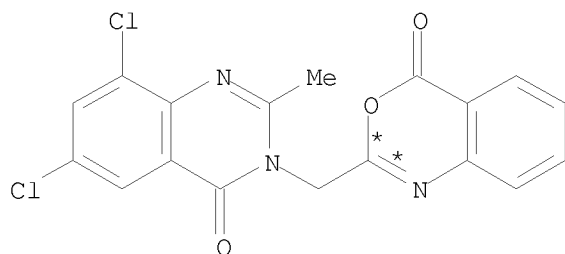
RX(37) OF 78 ...BG ==> BH



BG

(37) →

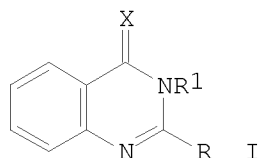
10/ 562,112



BH

RX(37)      RCT    BG 122418-03-5  
             PRO    BH 122418-04-6  
             CAT    108-24-7 Ac2O

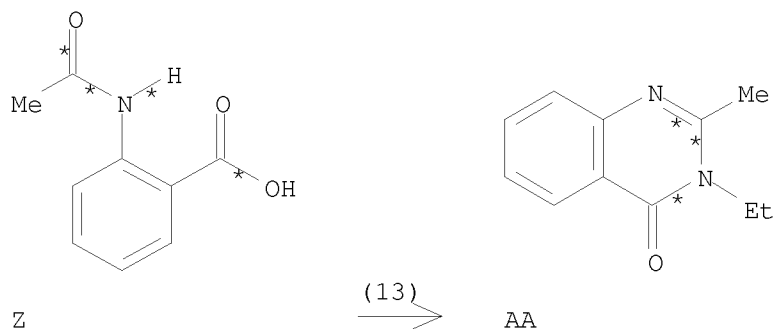
L3    ANSWER 166 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER:      111:97171    CASREACT  
TITLE:                    Studies on some biologically active  
                             azepinoquinazolines. Part I. An approach to potent  
                             bronchodilatory compounds  
AUTHOR(S):                Malhotra, S.; Koul, S. K.; Sharma, R. L.; Anand, K.  
                             K.; Gupta, O. P.; Dhar, K. L.  
CORPORATE SOURCE:        Nat. Prod. Chem. Div., Reg. Res. Lab., Jammu Tawi, 180  
                             001, India  
SOURCE:                    Indian Journal of Chemistry, Section B: Organic  
                             Chemistry Including Medicinal Chemistry (1988),  
                             27B(10), 937-40  
                             CODEN: IJSBDB; ISSN: 0376-4699  
DOCUMENT TYPE:            Journal  
LANGUAGE:                  English  
GI



AB    Quinazolines I [X = O, H<sub>2</sub>; RR<sub>1</sub> = (CH<sub>2</sub>)<sub>n</sub>; n = 3-9; R = Me, Et; R<sub>1</sub> = CHMe<sub>2</sub>, Pr, Bu, pentyl] have been prepared and screened for their bronchodilatory activity. I [X = O, RR<sub>1</sub> = (CH<sub>2</sub>)<sub>5</sub>] has excellent bronchodilatory properties. 2,4,6-Tribromo-7,8,9,10-tetrahydroazepino[2,1-b]quinazolin 12(6H)-one, prepared by brominating I [X = O, RR<sub>1</sub> = (CH<sub>2</sub>)<sub>5</sub>], shows marked antitussive and mucolytic activities parallel to those of bromhexine.

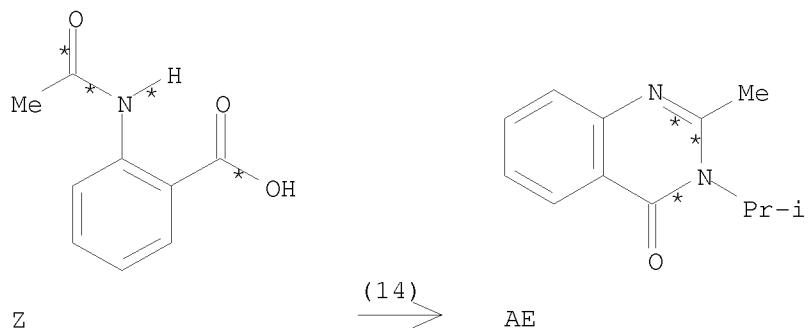
RX(13) OF 25      Z    ==>    AA

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RX(13)     RCT    Z 89-52-1  
             RGT    AB 75-04-7 EtNH2  
             PRO    AA 50677-59-3  
             CAT    110-86-1 Pyridine  
             SOL    71-43-2 Benzene

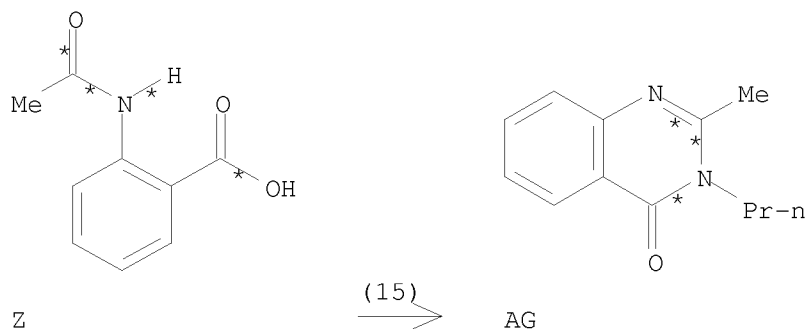
RX(14) OF 25     Z    ==>    AE



RX(14)     RCT    Z 89-52-1  
             RGT    AF 75-31-0 i-PrNH2  
             PRO    AE 10367-29-0  
             CAT    110-86-1 Pyridine  
             SOL    71-43-2 Benzene

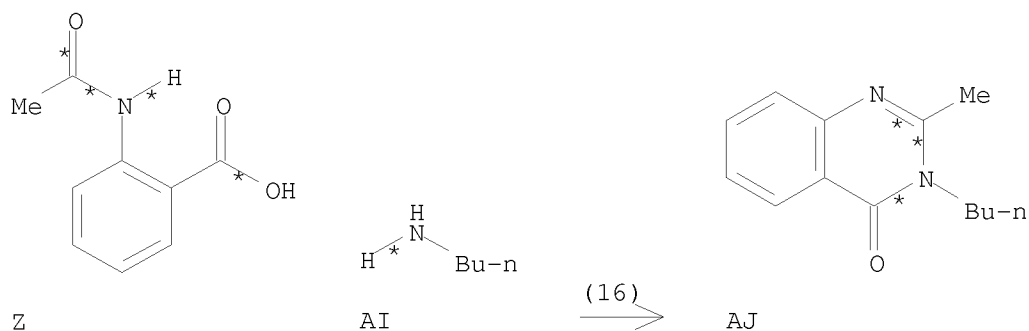
RX(15) OF 25     Z    ==>    AG

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RX(15)     RCT   Z 89-52-1  
           RGT   AH 107-10-8 PrNH2  
           PRO   AG 50677-60-6  
           CAT   110-86-1 Pyridine  
           SOL   71-43-2 Benzene

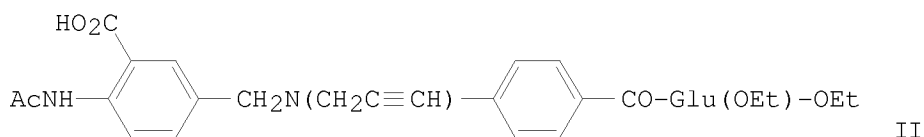
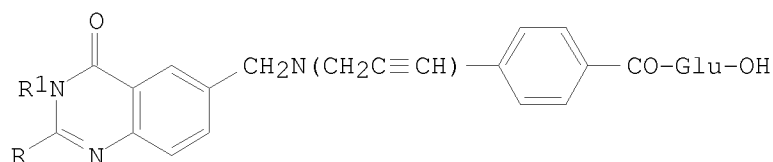
RX(16) OF 25     Z   +   AI   ==>   AJ



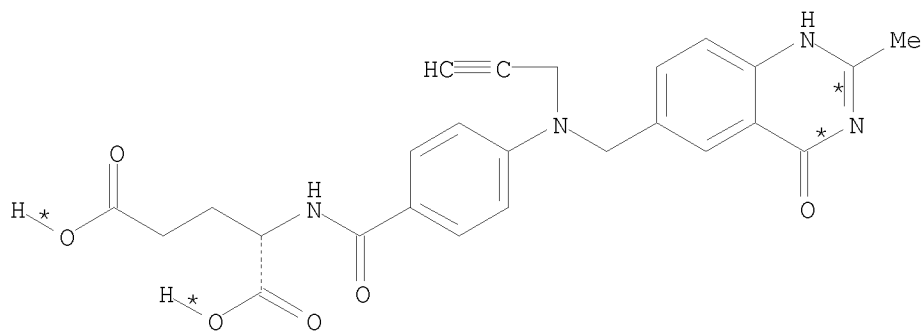
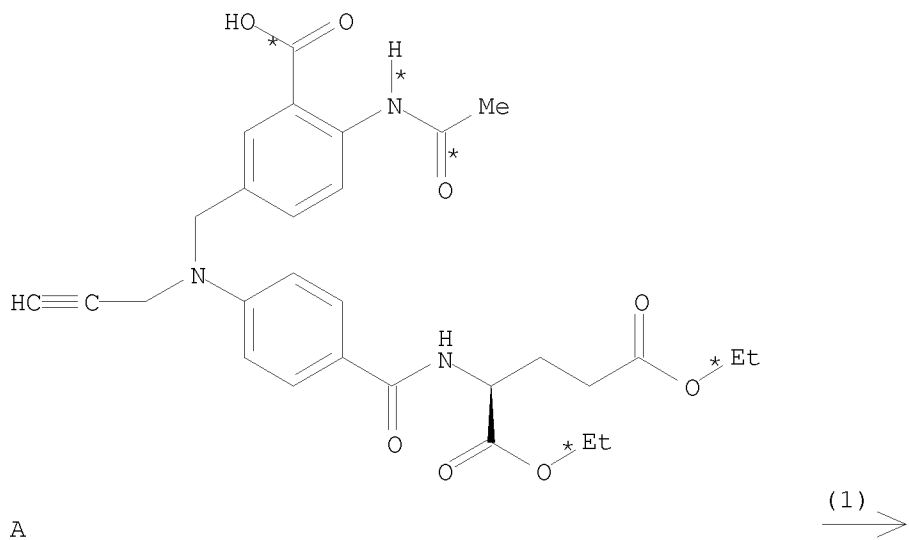
RX(16)     RCT   Z 89-52-1, AI 109-73-9  
           RGT   AC 110-86-1 Pyridine  
           PRO   AJ 394-90-1  
           SOL   71-43-2 Benzene

L3     ANSWER 167 OF 258     CASREACT     COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER:     110:232041     CASREACT  
TITLE:     Folate analogs. 32. Synthesis and biological  
           evaluation of 2-desamino-2-methyl-N10-propargyl-5,8-  
           dideazafolic acid and related compounds  
AUTHOR(S):     Patil, Sharadbala D.; Jones, Cecil; Nair, M. G.;  
           Galivan, J.; Maley, F.; Kisliuk, R. L.; Gaumont, Y;  
           Duch, David; Ferone, Robert  
CORPORATE SOURCE:     Dep. Biochem., Univ. South Alabama, Mobile, AL, 36688,  
           USA  
SOURCE:     Journal of Medicinal Chemistry (1989), 32(6), 1284-9





AB The chemical synthesis of 3 close analogs I ( $R = \text{Me}$ ,  $R_1 = \text{H}$ ,  $\text{Me}$ ;  $R = \text{CF}_3$ ,  $R_1 = \text{H}$ ) of N10-propargyl-5,8-dideazafolate (I,  $R = \text{NH}_2$ ,  $R_1 = \text{H}$ ) (II) is described. The quinazoline ring of I ( $R = \text{Me}$ ,  $R_1 = \text{H}$ ,  $\text{Me}$ ) was constructed from the pivotal intermediate II in a novel and unambiguous manner during the final step of the synthesis under very mild conditions. I ( $R = \text{Me}$ ,  $R_1 = \text{H}$ ) (III) was a strong inhibitor of human and *Lactobacillus casei* thymidylate synthases, whereas I ( $R = R_1 = \text{Me}$ ;  $R = \text{CF}_3$ ,  $R_1 = \text{H}$ ) were only weak inhibitors of this enzyme. III exhibited excellent growth inhibition of Manca human lymphoid leukemia and H35 hepatoma cells in culture. The inhibitory activities of III were 43 and 65-fold greater than that of II, resp., in these cell lines. H35R cells that are resistant to methotrexate (MTX) by virtue of a transport defect were cross-resistant to III but not to II. H35FF cells which have 70-fold greater amts. of thymidylate synthase compared to H35N cells were 130-fold resistant to III. Furthermore, the toxicity of III to H35 hepatoma cells could be completely reversed by thymidine, establishing its locus of action as thymidylate synthase. Transport studies in vitro established that III effectively inhibits MTX influx into H35 hepatoma cells, whereas II has no effect on MTX transport in this cell line. These data suggest that the greater activity of III relative to II is partly due to the ability of the former compound to enter cells via the MTX/reduced folate transport system.



B  
YIELD 46%

```

RX(1)          RCT   A 119820-58-5

                STAGE(1)
                RGT   C 109-02-4 N-Methylmorpholine, D 543-27-1 ClCO2Bu-i
                SOL   68-12-2 DMF

                STAGE(2)
                RGT   E 7664-41-7 NH3
                SOL   68-12-2 DMF

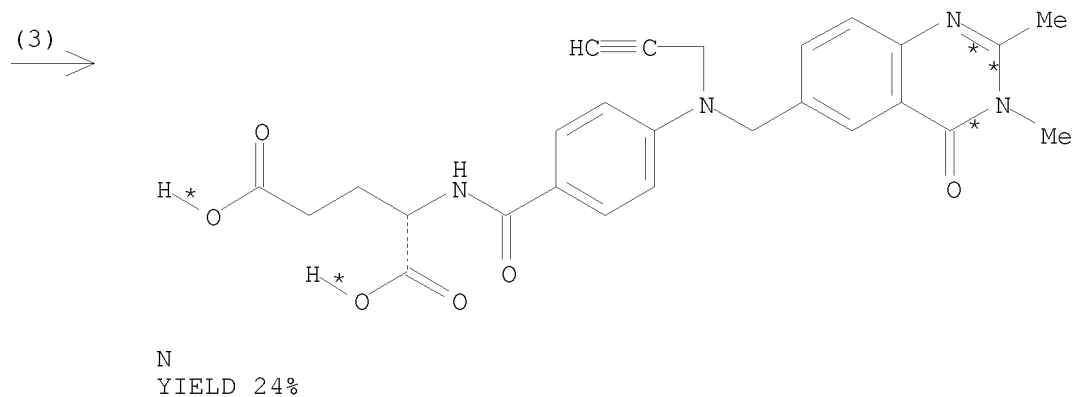
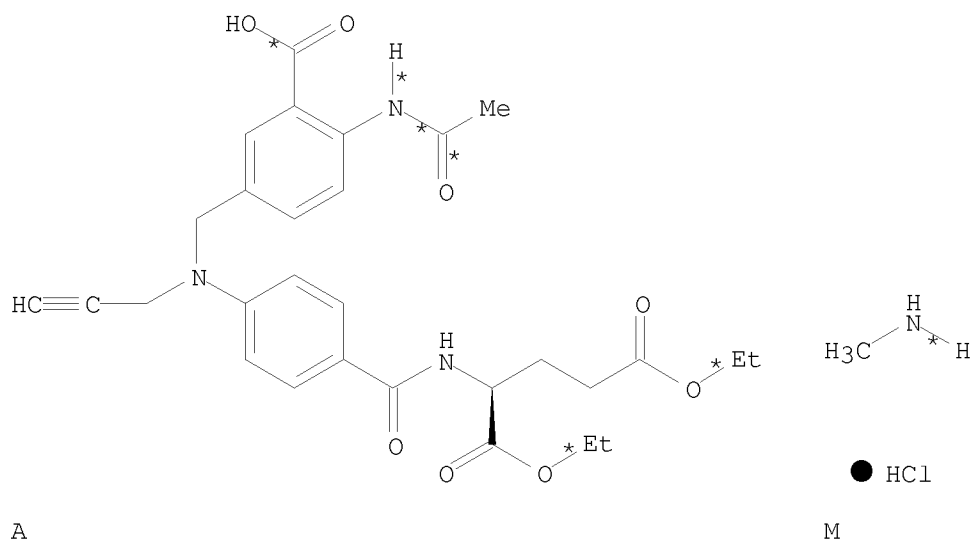
                STAGE(3)
                RGT   F 1310-73-2 NaOH
                SOL   7732-18-5 Water, 75-05-8 MeCN

PRO   B 112887-62-4

```

$$RX(3) \text{ OF } 38 \quad \dots A + M \implies N$$

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RX(3) RCT A 119820-58-5

STAGE(1)

RGT C 109-02-4 N-Methylmorpholine, D 543-27-1 ClCO<sub>2</sub>Bu-i

SOL 68-12-2 DMF

STAGE(2)

RCT M 593-51-1

RGT O 121-44-8 Et<sub>3</sub>N

SOL 68-12-2 DMF

STAGE(3)

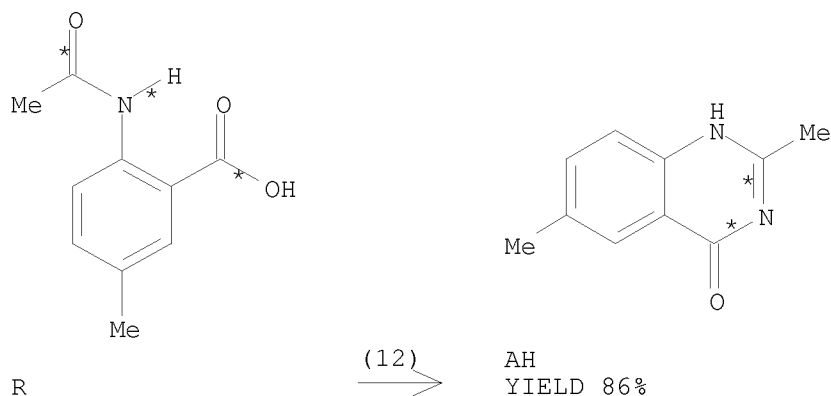
RGT F 1310-73-2 NaOH

SOL 7732-18-5 Water, 75-05-8 MeCN

PRO N 119820-56-3

RX(12) OF 38 ...R ==> AH...

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RX(12) RCT R 67081-68-9

STAGE(1)

RGT C 109-02-4 N-Methylmorpholine, D 543-27-1 ClCO<sub>2</sub>Bu-i  
SOL 68-12-2 DMF

STAGE(2)

RGT E 7664-41-7 NH<sub>3</sub>  
SOL 68-12-2 DMF

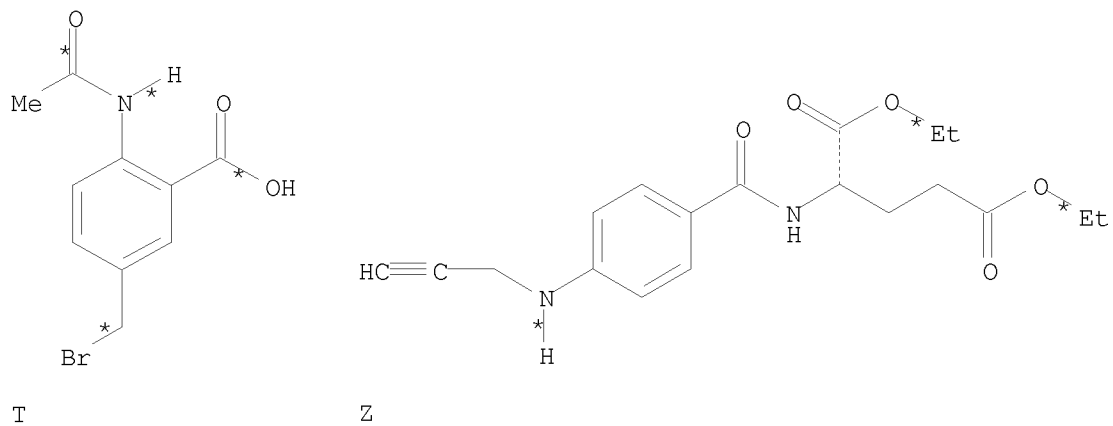
STAGE(3)

RGT F 1310-73-2 NaOH  
SOL 7732-18-5 Water, 75-05-8 MeCN

PRO AH 18731-19-6

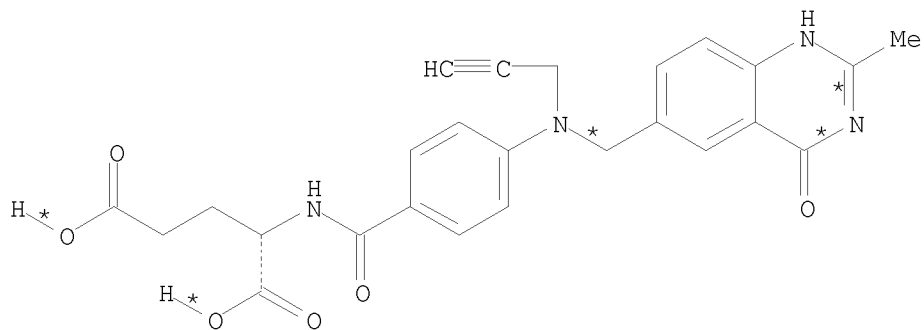
RX(17) OF 38 COMPOSED OF RX(7), RX(1)

RX(17) T + Z ==> B



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2  
STEPS  
→



B  
YIELD 46%

RX(7)	RCT	T 119820-57-4, Z 76858-72-5
	RGT	AA 1309-48-4 MgO
	PRO	A 119820-58-5
	SOL	127-19-5 AcNMe2

RX (1) RCT A 119820-58-5

STAGE ( 1 )

RGT C 109-02-4 N-Methylmorpholine, D 543-27-1 ClCO2Bu-i  
SOL 68-12-2 DMF

STAGE (2)

RGT E 7664-41-7 NH3  
SOL 68-12-2 DMF

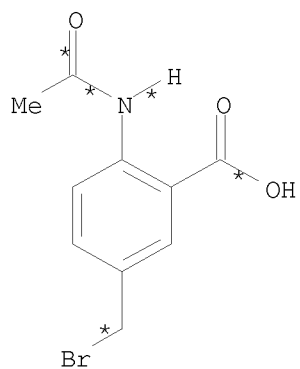
### STAGE (3)

RGT F 1310-73-2 NaOH  
SOL 7732-18-5 Water, 75-05-8 MeCN

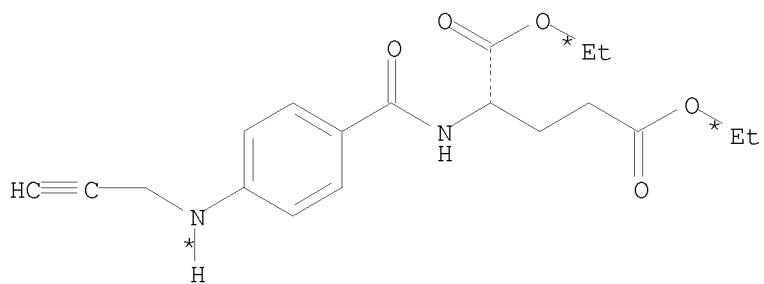
PRO B 112887-62-4

$$\begin{array}{l} \text{RX(18) OF 38 COMPOSED OF RX(7), RX(3)} \\ \text{RX(18) T + Z + M ==> N} \end{array}$$

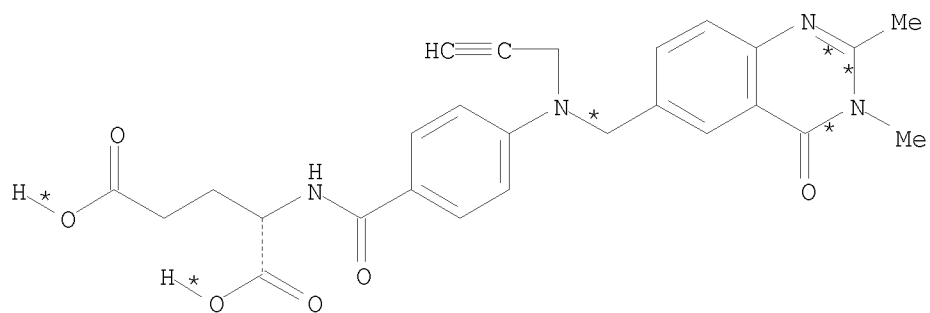
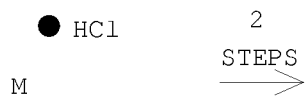
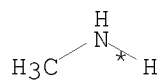
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T



Z



N

YIELD 24%

RX(7) RCT T 119820-57-4, Z 76858-72-5

RGT AA 1309-48-4 MgO

PRO A 119820-58-5

SOL 127-19-5 AcNMe2

RX(3) RCT A 119820-58-5

STAGE(1)

RGT C 109-02-4 N-Methylmorpholine, D 543-27-1 ClCO2Bu-i

SOL 68-12-2 DMF

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STAGE(2)

RCT M 593-51-1  
RGT O 121-44-8 Et3N  
SOL 68-12-2 DMF

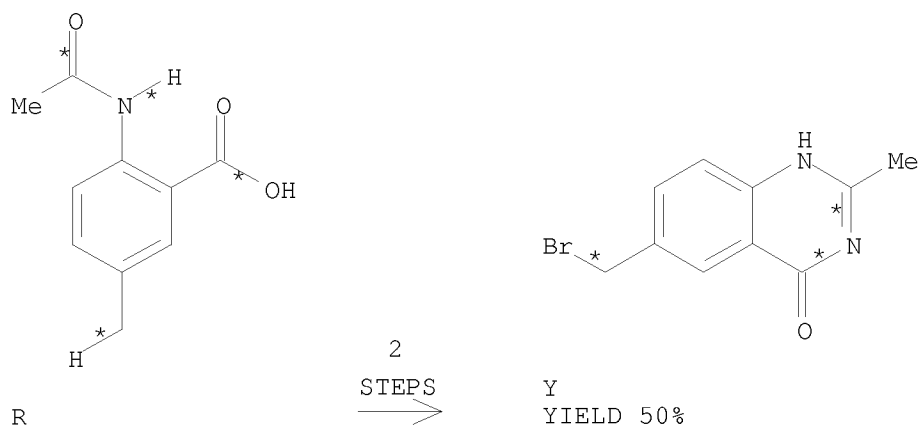
STAGE(3)

RGT F 1310-73-2 NaOH  
SOL 7732-18-5 Water, 75-05-8 MeCN

PRO N 119820-56-3

RX(23) OF 38 COMPOSED OF RX(12), RX(13)

RX(23) R ==> Y



RX(12) RCT R 67081-68-9

STAGE(1)

RGT C 109-02-4 N-Methylmorpholine, D 543-27-1 ClCO2Bu-i  
SOL 68-12-2 DMF

STAGE(2)

RGT E 7664-41-7 NH3  
SOL 68-12-2 DMF

STAGE(3)

RGT F 1310-73-2 NaOH  
SOL 7732-18-5 Water, 75-05-8 MeCN

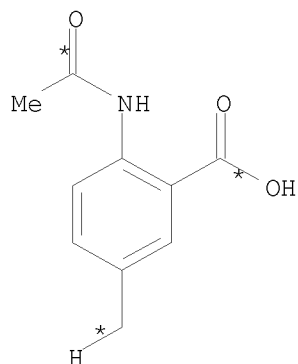
PRO AH 18731-19-6

RX(13) RCT AH 18731-19-6  
RGT U 77-48-5 Br2-Me2-hydantoin  
PRO Y 112888-43-4  
CAT 94-36-0 Benzoyl peroxide  
SOL 56-23-5 CCl4, 67-66-3 CHCl3  
NTE Photochem.

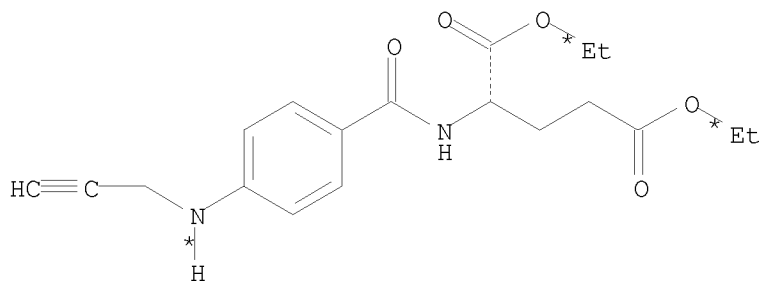
RX(27) OF 38 COMPOSED OF RX(5), RX(7), RX(1)

RX(27) R + Z ==> B

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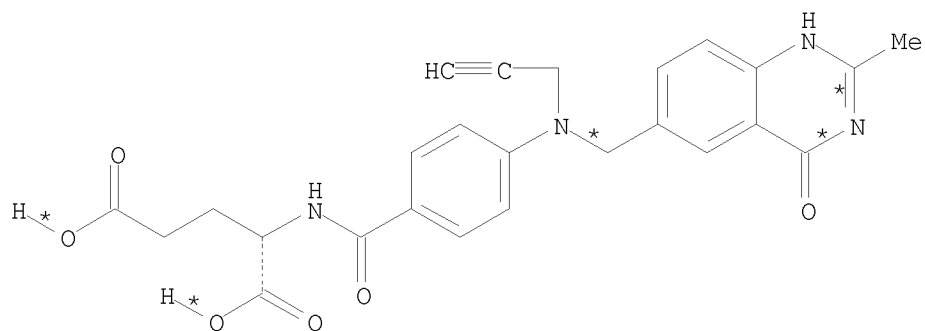


R



Z

3  
STEPS  
→



B  
YIELD 46%

RX(5)      RCT    R 67081-68-9  
             RGT    U 77-48-5 Br2-Me2-hydantoin  
             PRO    T 119820-57-4  
             CAT    94-36-0 Benzoyl peroxide  
             SOL    67-66-3 CHCl3, 56-23-5 CCl4  
             NTE    Photochem.

RX(7)      RCT    T 119820-57-4, Z 76858-72-5  
             RGT    AA 1309-48-4 MgO  
             PRO    A 119820-58-5  
             SOL    127-19-5 AcNMe2

RX(1)      RCT    A 119820-58-5

STAGE(1)

RGT    C 109-02-4 N-Methylmorpholine, D 543-27-1 ClCO2Bu-i



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SOL 68-12-2 DMF

STAGE(2)

RGT E 7664-41-7 NH3

SOL 68-12-2 DMF

STAGE(3)

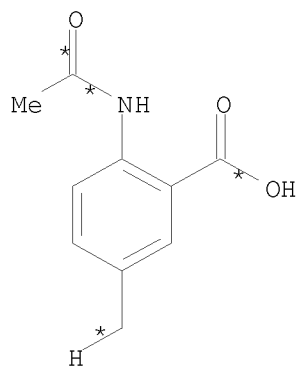
RGT F 1310-73-2 NaOH

SOL 7732-18-5 Water, 75-05-8 MeCN

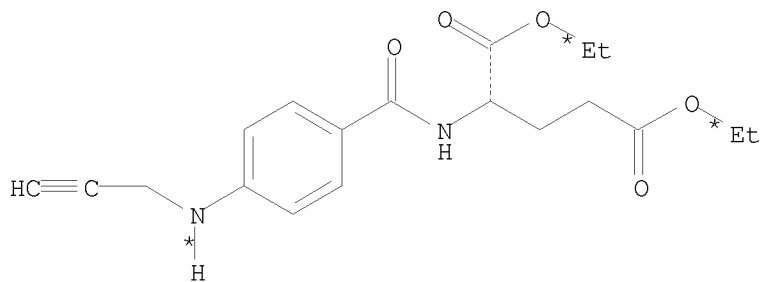
PRO B 112887-62-4

RX(28) OF 38 COMPOSED OF RX(5), RX(7), RX(3)

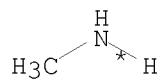
RX(28) R + Z + M ==> N



R



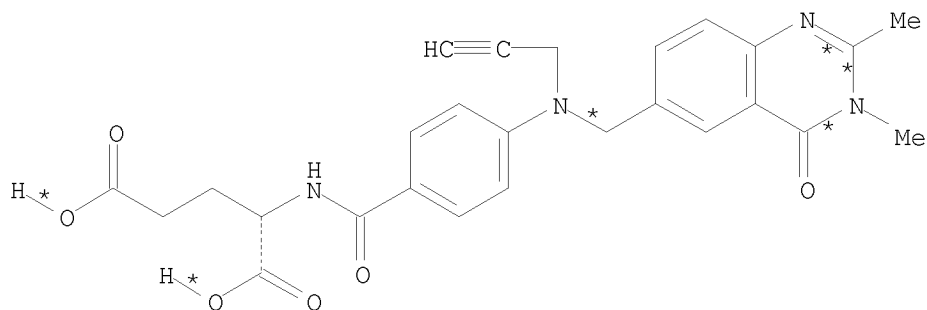
Z



M

● HCl

3  
STEPS  
→



N  
YIELD 24%

RX(5)	RCT	R 67081-68-9
	RGT	U 77-48-5 Br2-Me2-hydantoin
	PRO	T 119820-57-4
	CAT	94-36-0 Benzoyl peroxide
	SOL	67-66-3 CHCl3, 56-23-5 CCl4
	NTE	Photochem.

RX(7)	RCT	T 119820-57-4, Z 76858-72-5
	RGT	AA 1309-48-4 MgO
	PRO	A 119820-58-5
	SOL	127-19-5 AcNMe2

RX (3)            RCT    A 119820-58-5

STAGE (1)

RGT C 109-02-4 N-Methylmorpholine, D 543-27-1 ClCO2Bu-i  
SOL 68-12-2 DMF

## STAGE (2)

RCT M 593-51-1  
RGT O 121-44-8 Et3N  
SOL 68-12-2 DMF

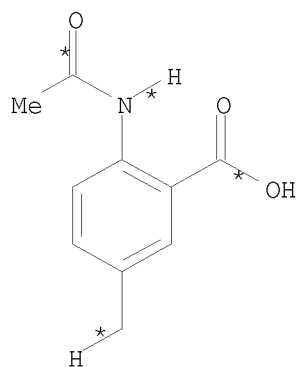
### STAGE (3)

RGT F 1310-73-2 NaOH  
SOL 7732-18-5 Water, 75-05-8 MeCN

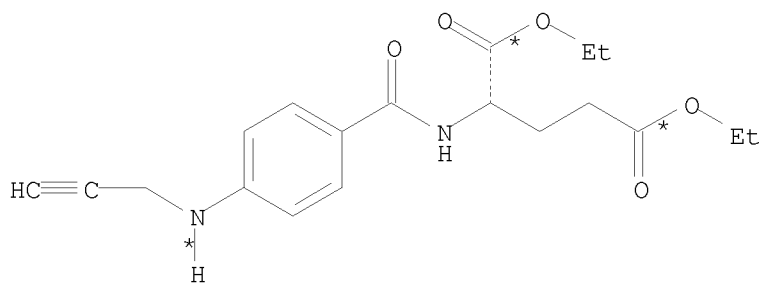
PRO N 119820-56-3

RX(36) OF 38 COMPOSED OF RX(12), RX(13), RX(6)  
 RX(36) R + Z ==> B

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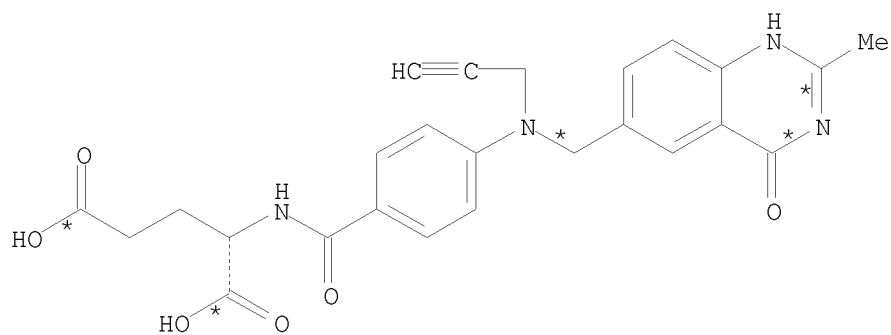


R



Z

3  
STEPS  
→



B

YIELD 67%

RX(12) RCT R 67081-68-9

STAGE(1)

RGT C 109-02-4 N-Methylmorpholine, D 543-27-1 ClCO<sub>2</sub>Bu-i  
SOL 68-12-2 DMF

STAGE(2)

RGT E 7664-41-7 NH<sub>3</sub>  
SOL 68-12-2 DMF

STAGE(3)

RGT F 1310-73-2 NaOH  
SOL 7732-18-5 Water, 75-05-8 MeCN

PRO AH 18731-19-6

RX(13) RCT AH 18731-19-6

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RGT U 77-48-5 Br2-Me2-hydantoin  
PRO Y 112888-43-4  
CAT 94-36-0 Benzoyl peroxide  
SOL 56-23-5 CCl4, 67-66-3 CHCl3  
NTE Photochem.

RX(6) RCT Y 112888-43-4, Z 76858-72-5

STAGE(1)

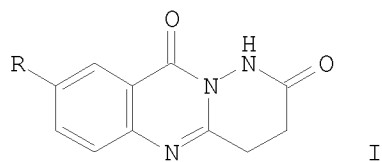
RGT AA 1309-48-4 MgO  
SOL 127-19-5 AcNMe2

STAGE(2)

RGT F 1310-73-2 NaOH  
SOL 7732-18-5 Water, 75-05-8 MeCN

PRO B 112887-62-4

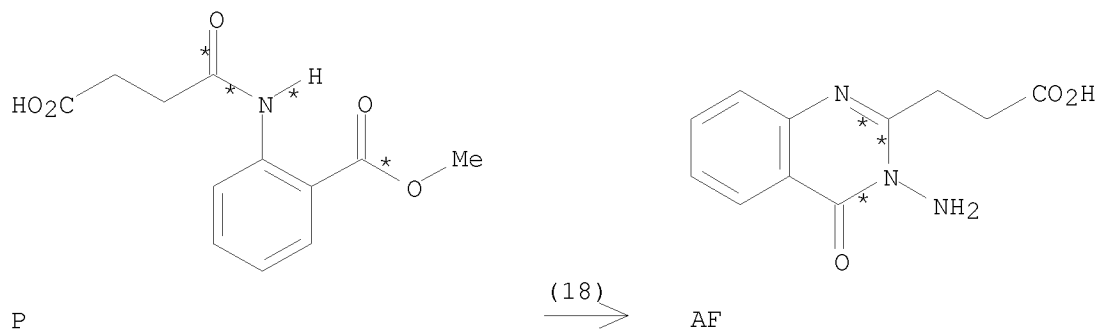
L3 ANSWER 168 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 110:212758 CASREACT  
TITLE: Reactions of cyclic anhydrides. Part XIII. Facile  
synthesis of 1,2,3,4-tetrahydro-10H-pyridazino[6,1-  
b]quinazoline-2,10-diones  
AUTHOR(S): Balasubramanian, V.; Argade, N. P.  
CORPORATE SOURCE: Sci. Res. cent., HPT Arts RYK Sci. Coll., Nashik, 422  
005, India  
SOURCE: Indian Journal of Chemistry, Section B: Organic  
Chemistry Including Medicinal Chemistry (1988),  
27B(10), 906-8  
CODEN: IJSBDB; ISSN: 0376-4699  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Pyridazinoquinazolin-2,10-diones I (R = H, B) have been prepared by hydrazinolysis of 4,2-R(R1O2C)C6H3NHCOCH2CH2CO2R2 (R1 = Me, Et, R2 = H, Me, Et) or alkyl  $\beta$ -(4-oxo-3,1-benzoxazin-2-yl)propionates via alkyl  $\beta$ -(3-amino-4-oxoquinazolin-2-yl)propionates or  $\beta$ -(3-amino-4-oxoquinazolin-2-yl)propionic hydrazide. I (R = H) has also been obtained by refluxing 2-H2NC6H4CONHNH2 and succinic anhydride in dry xylene.

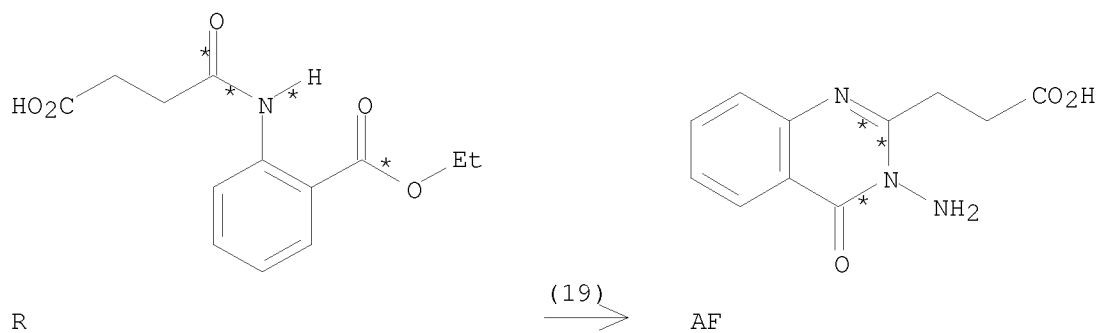
RX(18) OF 137 ...P ==> AF...

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RX(18)    RCT    P 108540-96-1  
              RGT    AG 302-01-2 N2H4  
              PRO    AF 84312-90-3  
              SOL    64-17-5 EtOH

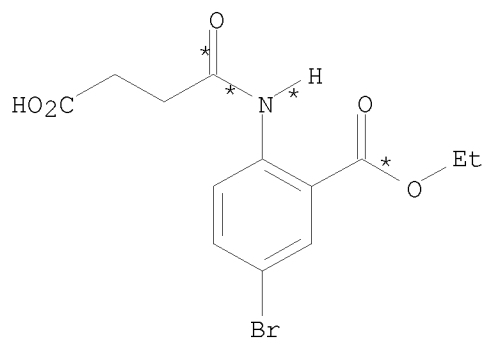
RX(19) OF 137    ...R    ==>    AF...



RX(19)    RCT    R 120572-38-5  
              RGT    AG 302-01-2 N2H4  
              PRO    AF 84312-90-3  
              SOL    64-17-5 EtOH

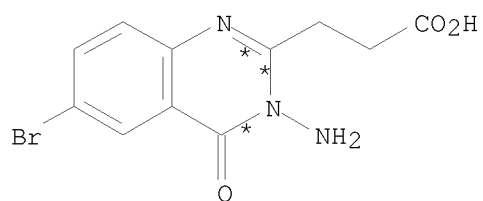
RX(20) OF 137    ...V    ==>    AH...

10/ 562,112



V

(20)  $\Rightarrow$

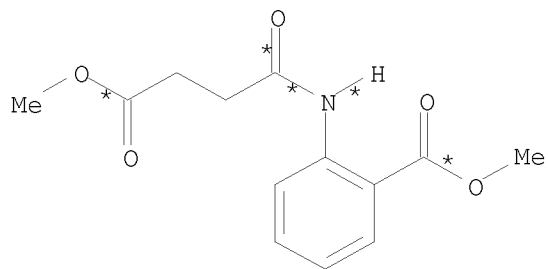


AH

YIELD 90%

RX(20)      RCT    V 120572-40-9  
              RGT    AG 302-01-2 N2H4  
              PRO    AH 120572-47-6  
              SOL    64-17-5 EtOH

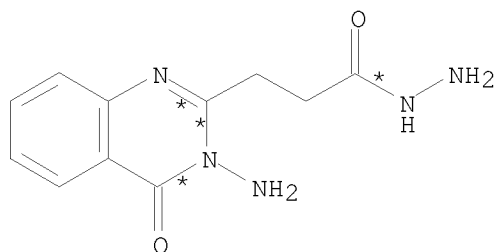
RX(24) OF 137      ...W ==> AL...



W

(24)  $\Rightarrow$

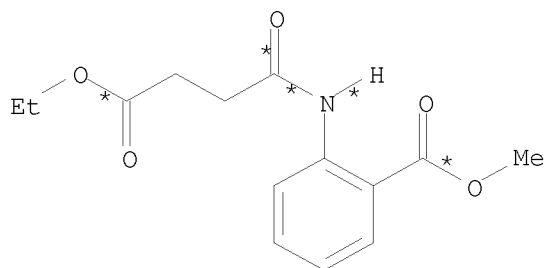
10/ 562,112



AL

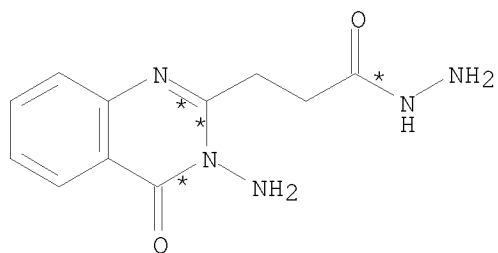
RX(24)      RCT    W 59868-50-7  
              RGT    AG 302-01-2 N2H4  
              PRO    AL 120572-51-2  
              SOL    64-17-5 EtOH

RX(25) OF 137      ...X    ==>    AL...



X

(25)  
→

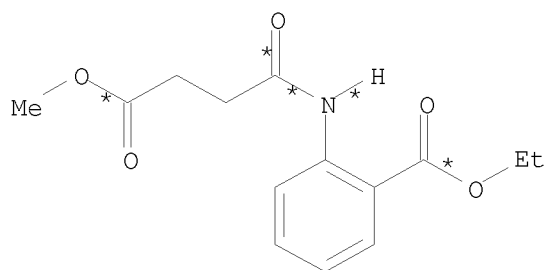


AL

RX(25)      RCT    X 120572-41-0  
              RGT    AG 302-01-2 N2H4  
              PRO    AL 120572-51-2  
              SOL    64-17-5 EtOH

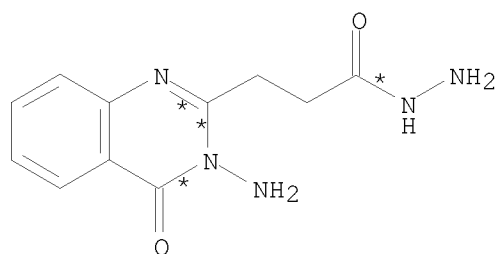
10/ 562,112

RX(26) OF 137      ...Y    ==>    AL...



Y

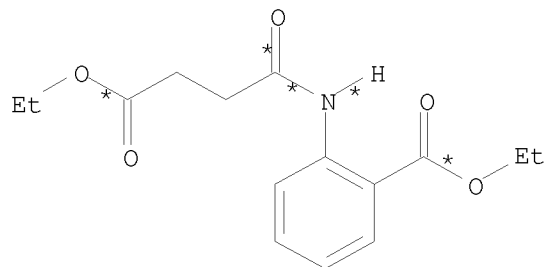
(26)



AL

RX(26)      RCT    Y 120572-42-1  
             RGT    AG 302-01-2 N2H4  
             PRO    AL 120572-51-2  
             SOL    64-17-5 EtOH

RX(27) OF 137      ...Z    ==>    AL...

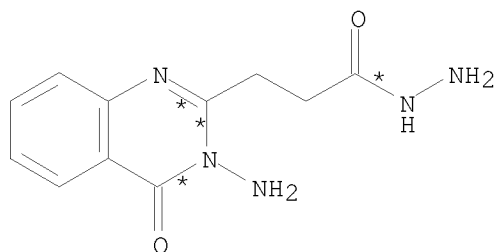


Z

(27)



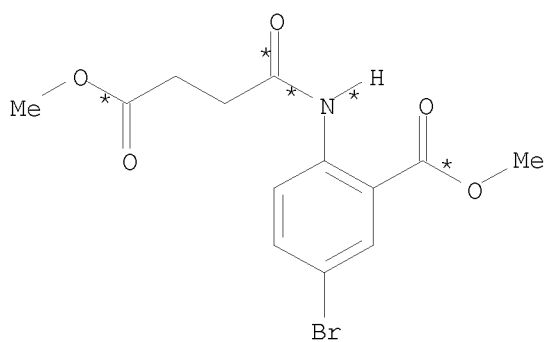
10/ 562,112



AL

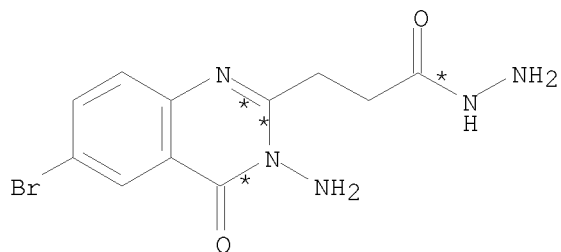
RX(27)      RCT    Z 120572-43-2  
             RGT    AG 302-01-2 N2H4  
             PRO    AL 120572-51-2  
             SOL    64-17-5 EtOH

RX(32) OF 137      ...AA ==> AM



AA

(32) →

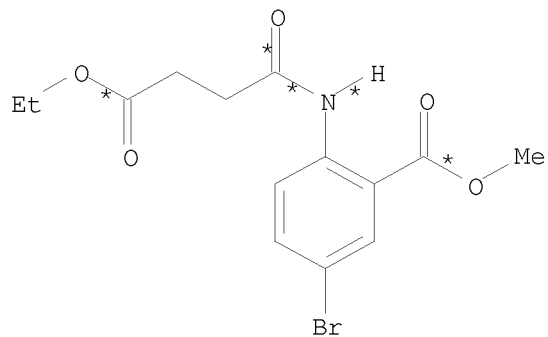


AM

RX(32)      RCT    AA 120572-44-3  
             RGT    AG 302-01-2 N2H4  
             PRO    AM 120572-52-3  
             SOL    64-17-5 EtOH

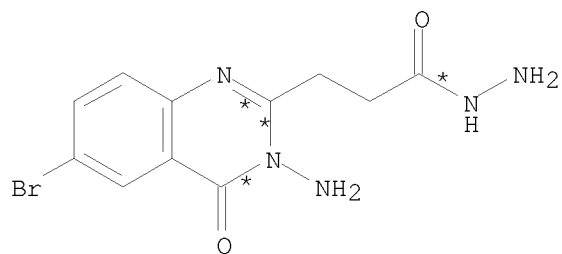
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RX(33) OF 137 ...AB ==> AM



AB

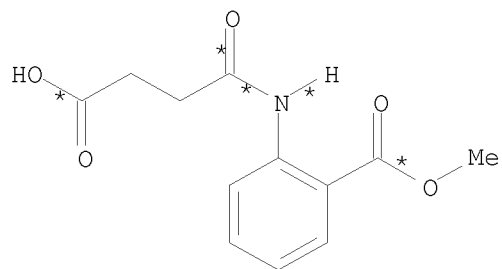
(33) 



AM

RX(33)      RCT    AB 120572-45-4  
              RGT    AG 302-01-2 N2H4  
              PRO    AM 120572-52-3  
              SOL    64-17-5 EtOH

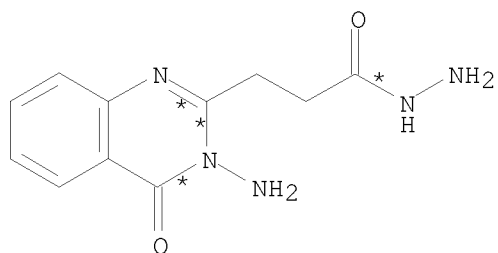
RX(53) OF 137 COMPOSED OF RX(10), RX(24)  
RX(53)      P      ==>    AL



P

2  
STEPS 

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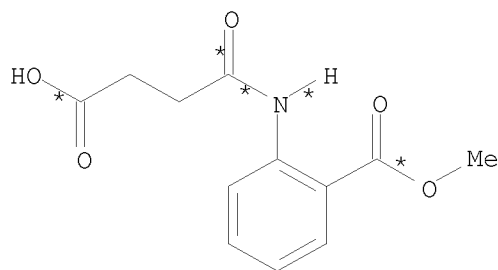


AL

RX(10)      RCT    P 108540-96-1  
              RGT    J 67-56-1 MeOH  
              PRO    W 59868-50-7  
              CAT    7664-93-9 H2SO4  
              SOL    67-56-1 MeOH

RX(24)      RCT    W 59868-50-7  
              RGT    AG 302-01-2 N2H4  
              PRO    AL 120572-51-2  
              SOL    64-17-5 EtOH

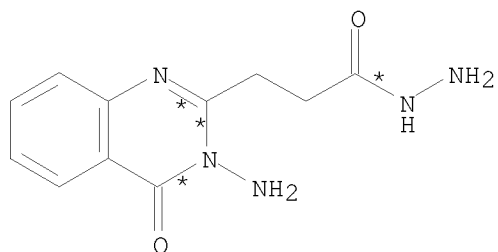
RX(54) OF 137 COMPOSED OF RX(11), RX(25)  
RX(54)      P      ==>    AL



P

2  
STEPS  
→

10/ 562,112

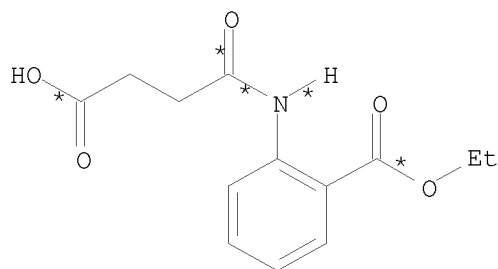


AL

RX(11)      RCT    P 108540-96-1  
              RGT    M 64-17-5 EtOH  
              PRO    X 120572-41-0  
              CAT    7664-93-9 H2SO4  
              SOL    64-17-5 EtOH

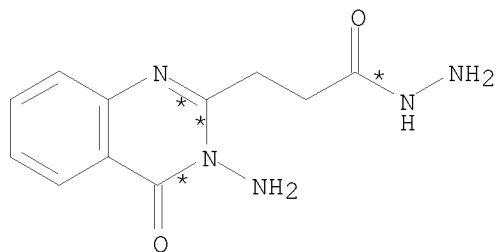
RX(25)      RCT    X 120572-41-0  
              RGT    AG 302-01-2 N2H4  
              PRO    AL 120572-51-2  
              SOL    64-17-5 EtOH

RX(55) OF 137 COMPOSED OF RX(12), RX(26)  
RX(55)      R    ==>    AL



R

2  
STEPS  
→



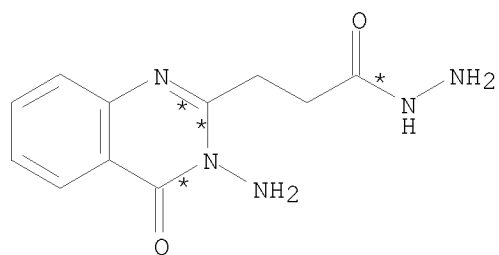
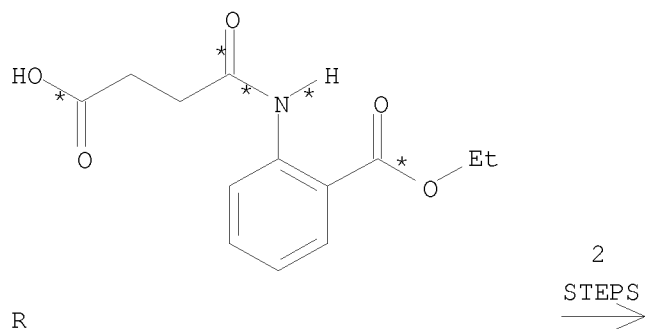
AL

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RX(12)      RCT    R 120572-38-5  
              RGT    J 67-56-1 MeOH  
              PRO    Y 120572-42-1  
              CAT    7664-93-9 H2SO4  
              SOL    67-56-1 MeOH

RX(26)      RCT    Y 120572-42-1  
              RGT    AG 302-01-2 N2H4  
              PRO    AL 120572-51-2  
              SOL    64-17-5 EtOH

RX(56) OF 137 COMPOSED OF RX(13), RX(27)  
RX(56)      R    ==>    AL



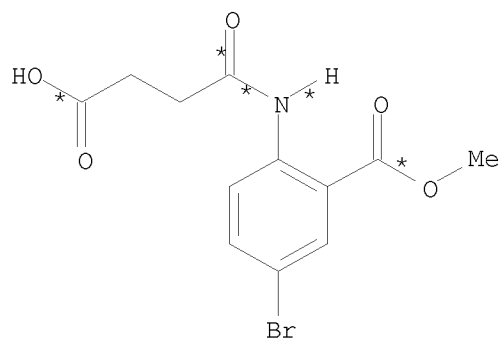
RX(13)      RCT    R 120572-38-5  
              RGT    M 64-17-5 EtOH  
              PRO    Z 120572-43-2  
              CAT    7664-93-9 H2SO4  
              SOL    64-17-5 EtOH

RX(27)      RCT    Z 120572-43-2  
              RGT    AG 302-01-2 N2H4  
              PRO    AL 120572-51-2  
              SOL    64-17-5 EtOH

RX(57) OF 137 COMPOSED OF RX(14), RX(32)

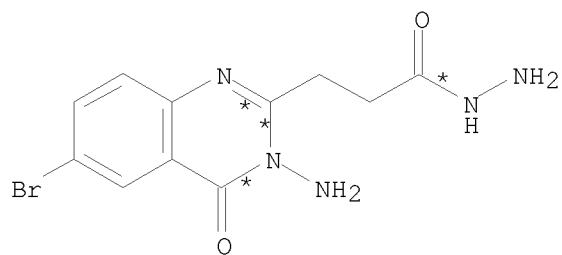
10/ 562,112

RX(57)      T    ==>    AM



T

2  
STEPS  
➔



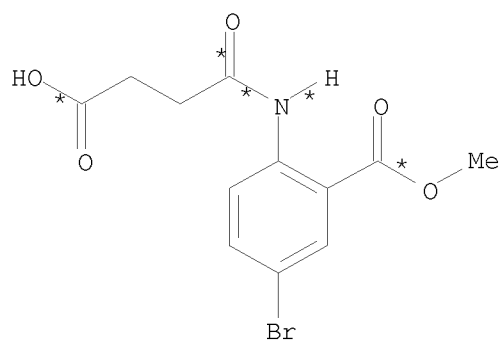
AM

RX(14)      RCT    T 120572-39-6  
              RGT    J 67-56-1 MeOH  
              PRO    AA 120572-44-3  
              CAT    7664-93-9 H2SO4  
              SOL    67-56-1 MeOH

RX(32)      RCT    AA 120572-44-3  
              RGT    AG 302-01-2 N2H4  
              PRO    AM 120572-52-3  
              SOL    64-17-5 EtOH

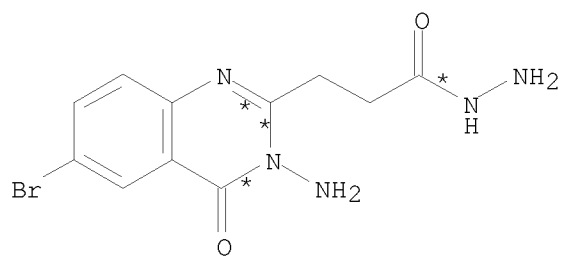
RX(58) OF 137 COMPOSED OF RX(15), RX(33)  
RX(58)      T    ==>    AM

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T

2  
STEPS  
→



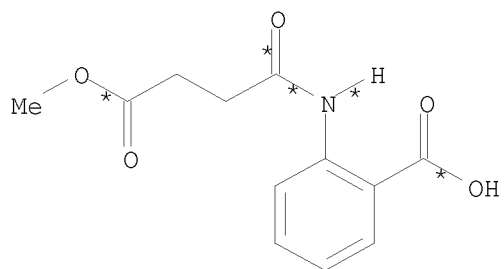
AM

RX(15)     RCT    T 120572-39-6  
             RGT    M 64-17-5 EtOH  
             PRO    AB 120572-45-4  
             CAT    7664-93-9 H2SO4  
             SOL    64-17-5 EtOH

RX(33)     RCT    AB 120572-45-4  
             RGT    AG 302-01-2 N2H4  
             PRO    AM 120572-52-3  
             SOL    64-17-5 EtOH

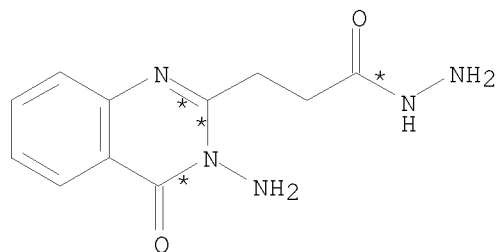
RX(59) OF 137 COMPOSED OF RX(16), RX(28)  
RX(59)     I     ==>    AL

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I

2  
STEPS  
→

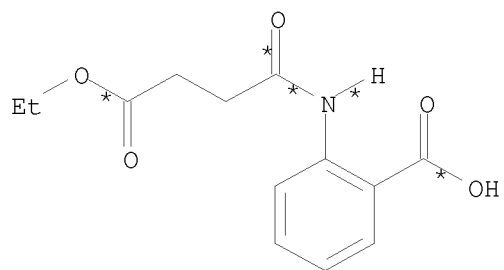


AL

RX(16)      RCT    I 54559-37-4  
              RGT    AD 108-24-7 Ac2O  
              PRO    AC 54559-36-3

RX(28)      RCT    AC 54559-36-3  
              RGT    AG 302-01-2 N2H4  
              PRO    AL 120572-51-2  
              SOL    64-17-5 EtOH

RX(60) OF 137 COMPOSED OF RX(17), RX(29)  
RX(60)      L    ==>    AL

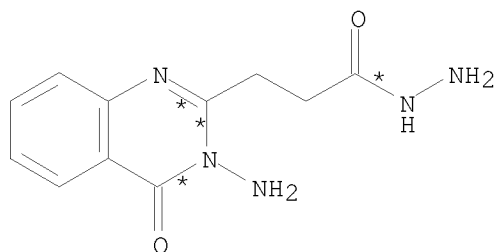


L

2  
STEPS  
→



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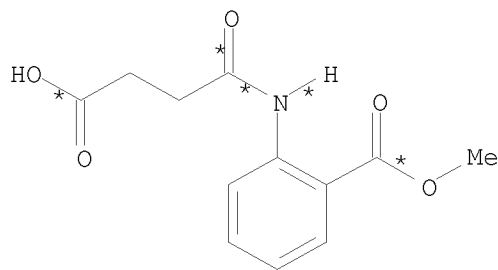


AL

RX(17) RCT L 120572-36-3  
RGT AD 108-24-7 Ac<sub>2</sub>O  
PRO AE 120572-46-5

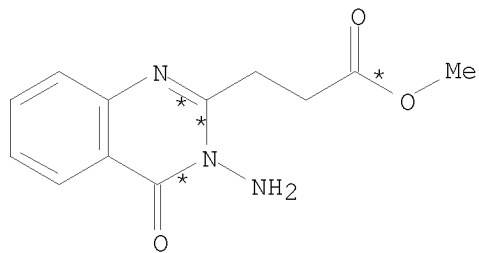
RX(29) RCT AE 120572-46-5  
RGT AG 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO AL 120572-51-2  
SOL 64-17-5 EtOH

RX(61) OF 137 COMPOSED OF RX(18), RX(21)  
RX(61) P ==> AI



P

2  
STEPS  
→



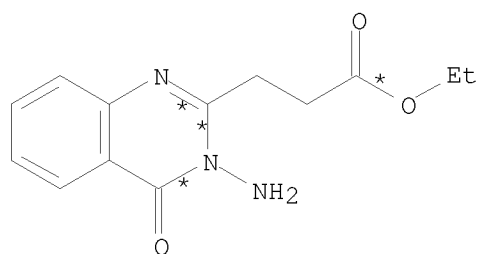
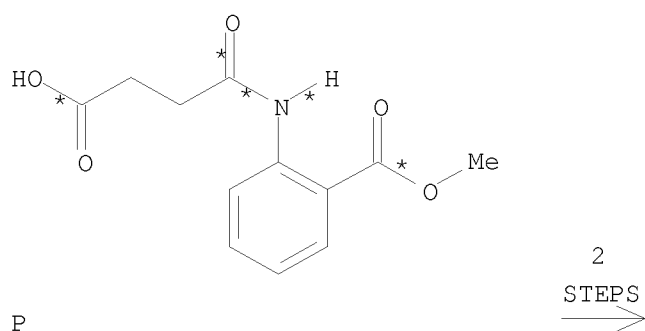
AI  
YIELD 80%

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RX(18)      RCT    P 108540-96-1  
              RGT    AG 302-01-2 N2H4  
              PRO    AF 84312-90-3  
              SOL    64-17-5 EtOH

RX(21)      RCT    AF 84312-90-3  
              RGT    J 67-56-1 MeOH  
              PRO    AI 120572-48-7  
              CAT    7664-93-9 H2SO4  
              SOL    67-56-1 MeOH

RX(62) OF 137 COMPOSED OF RX(18), RX(22)  
RX(62)      P    ==>    AJ



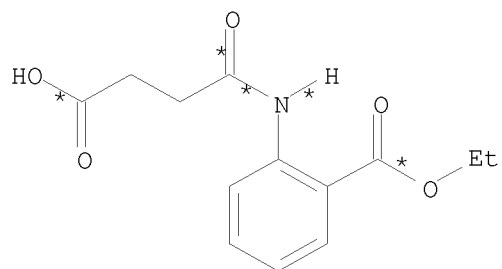
AJ  
YIELD 80%

RX(18)      RCT    P 108540-96-1  
              RGT    AG 302-01-2 N2H4  
              PRO    AF 84312-90-3  
              SOL    64-17-5 EtOH

RX(22)      RCT    AF 84312-90-3  
              RGT    M 64-17-5 EtOH  
              PRO    AJ 120572-49-8  
              CAT    7664-93-9 H2SO4  
              SOL    64-17-5 EtOH

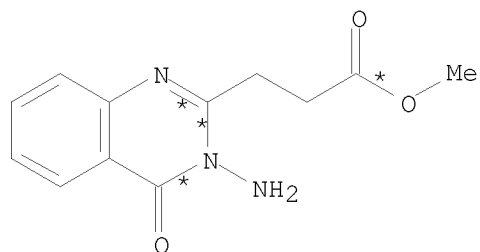
RX(63) OF 137 COMPOSED OF RX(19), RX(21)  
RX(63)      R    ==>    AI

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R

2  
STEPS  
→



AI

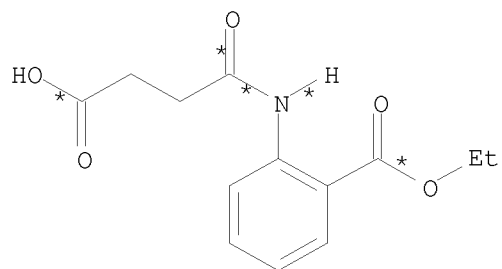
YIELD 80%

RX(19)     RCT   R 120572-38-5  
              RGT   AG 302-01-2 N2H4  
              PRO   AF 84312-90-3  
              SOL   64-17-5 EtOH

RX(21)     RCT   AF 84312-90-3  
              RGT   J 67-56-1 MeOH  
              PRO   AI 120572-48-7  
              CAT   7664-93-9 H2SO4  
              SOL   67-56-1 MeOH

RX(64) OF 137 COMPOSED OF RX(19), RX(22)

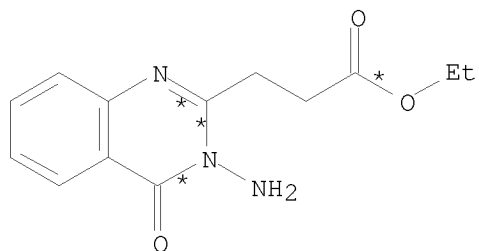
RX(64)     R   ==>   AJ



R

2  
STEPS  
→

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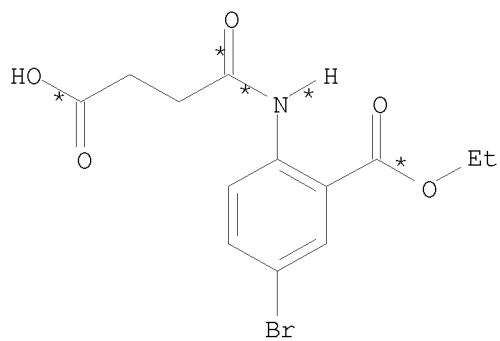


AJ  
YIELD 80%

RX(19)      RCT    R 120572-38-5  
              RGT    AG 302-01-2 N2H4  
              PRO    AF 84312-90-3  
              SOL    64-17-5 EtOH

RX(22)      RCT    AF 84312-90-3  
              RGT    M 64-17-5 EtOH  
              PRO    AJ 120572-49-8  
              CAT    7664-93-9 H2SO4  
              SOL    64-17-5 EtOH

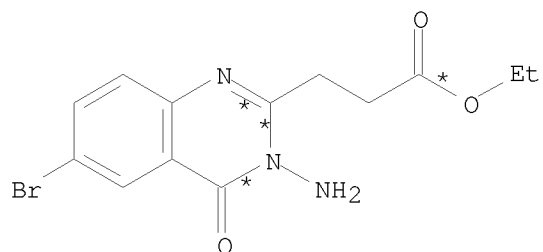
RX(65) OF 137 COMPOSED OF RX(20), RX(23)  
RX(65)      V      ==>    AK



V

2  
STEPS  
→

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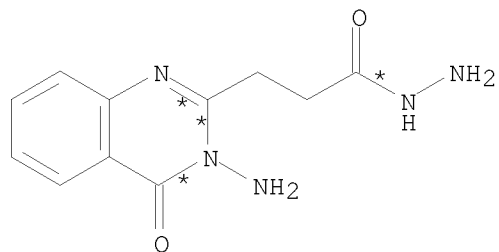
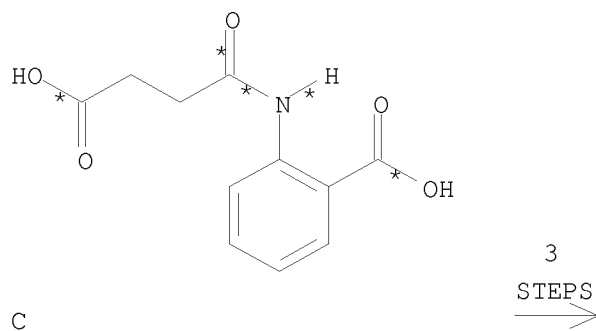


AK  
YIELD 85%

RX(20)      RCT    V 120572-40-9  
              RGT    AG 302-01-2 N2H4  
              PRO    AH 120572-47-6  
              SOL    64-17-5 EtOH

RX(23)      RCT    AH 120572-47-6  
              RGT    M 64-17-5 EtOH  
              PRO    AK 120572-50-1  
              CAT    7664-93-9 H2SO4  
              SOL    64-17-5 EtOH

RX(81) OF 137 COMPOSED OF RX(3), RX(16), RX(28)  
RX(81)      C    ==>    AL



AL

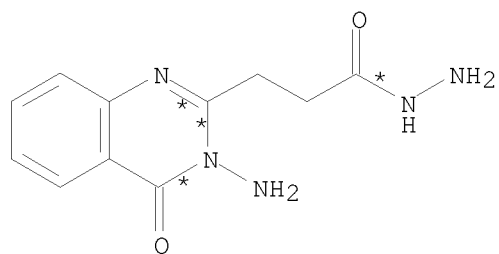
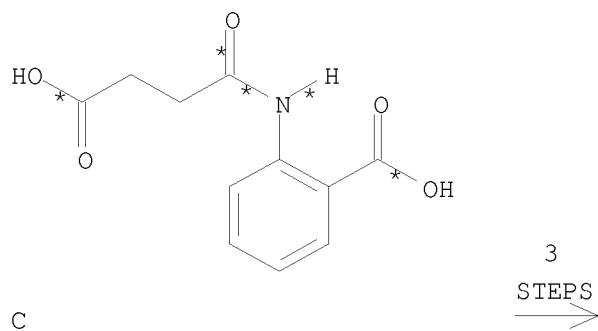
10/ 562,112

RX(3)      RCT    C 5694-37-1  
             RGT    J 67-56-1 MeOH  
             PRO    I 54559-37-4  
             CAT    7664-93-9 H2SO4  
             SOL    67-56-1 MeOH

RX(16)     RCT    I 54559-37-4  
             RGT    AD 108-24-7 Ac2O  
             PRO    AC 54559-36-3

RX(28)     RCT    AC 54559-36-3  
             RGT    AG 302-01-2 N2H4  
             PRO    AL 120572-51-2  
             SOL    64-17-5 EtOH

RX(83) OF 137 COMPOSED OF RX(4), RX(17), RX(29)  
RX(83)      C    ==>    AL



AL

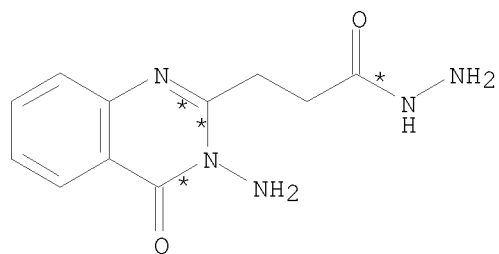
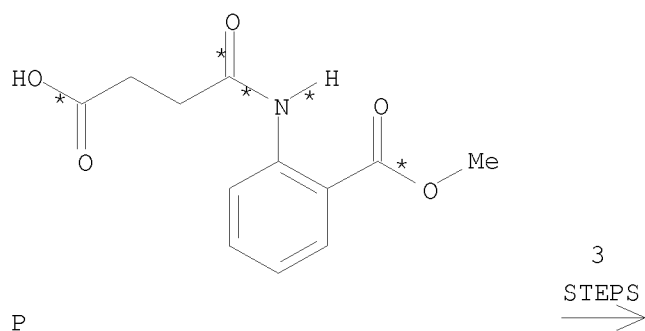
RX(4)      RCT    C 5694-37-1  
             RGT    M 64-17-5 EtOH  
             PRO    L 120572-36-3  
             CAT    7664-93-9 H2SO4  
             SOL    64-17-5 EtOH

RX(17)     RCT    L 120572-36-3  
             RGT    AD 108-24-7 Ac2O  
             PRO    AE 120572-46-5

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RX(29)      RCT    AE 120572-46-5  
              RGT    AG 302-01-2 N2H4  
              PRO    AL 120572-51-2  
              SOL    64-17-5 EtOH

RX(108) OF 137 COMPOSED OF RX(18), RX(21), RX(30)  
RX(108)    P    ==>    AL



AL

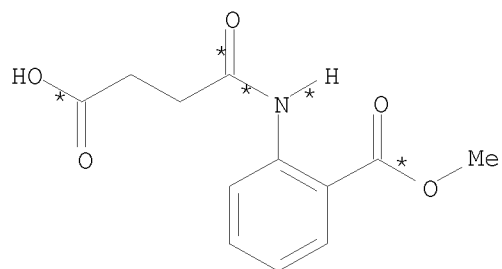
RX(18)      RCT    P 108540-96-1  
              RGT    AG 302-01-2 N2H4  
              PRO    AF 84312-90-3  
              SOL    64-17-5 EtOH

RX(21)      RCT    AF 84312-90-3  
              RGT    J 67-56-1 MeOH  
              PRO    AI 120572-48-7  
              CAT    7664-93-9 H2SO4  
              SOL    67-56-1 MeOH

RX(30)      RCT    AI 120572-48-7  
              RGT    AG 302-01-2 N2H4  
              PRO    AL 120572-51-2  
              SOL    64-17-5 EtOH

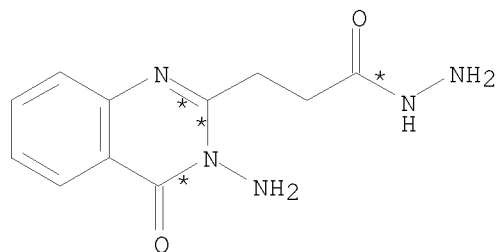
RX(110) OF 137 COMPOSED OF RX(18), RX(22), RX(31)  
RX(110)    P    ==>    AL

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P

3  
STEPS  
→



AL

RX(18)      RCT    P 108540-96-1  
              RGT    AG 302-01-2 N2H4  
              PRO    AF 84312-90-3  
              SOL    64-17-5 EtOH

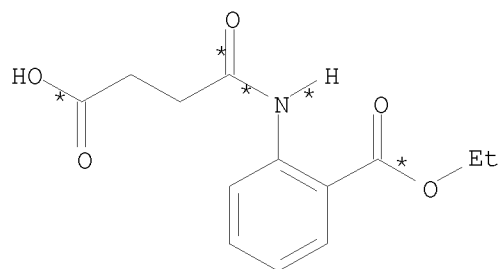
RX(22)      RCT    AF 84312-90-3  
              RGT    M 64-17-5 EtOH  
              PRO    AJ 120572-49-8  
              CAT    7664-93-9 H2SO4  
              SOL    64-17-5 EtOH

RX(31)      RCT    AJ 120572-49-8  
              RGT    AG 302-01-2 N2H4  
              PRO    AL 120572-51-2  
              SOL    64-17-5 EtOH

RX(112) OF 137 COMPOSED OF RX(19), RX(21), RX(30)  
RX(112)    R    ==>    AL

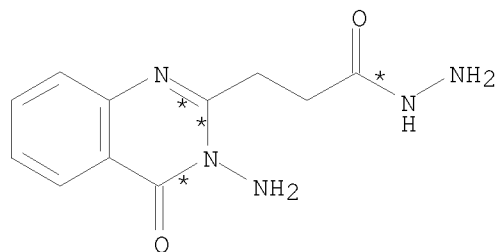


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R

3  
STEPS  
→



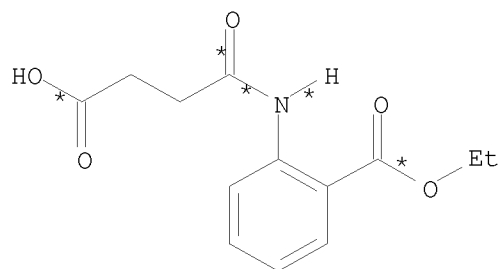
AL

RX(19)      RCT    R 120572-38-5  
              RGT    AG 302-01-2 N2H4  
              PRO    AF 84312-90-3  
              SOL    64-17-5 EtOH

RX(21)      RCT    AF 84312-90-3  
              RGT    J 67-56-1 MeOH  
              PRO    AI 120572-48-7  
              CAT    7664-93-9 H2SO4  
              SOL    67-56-1 MeOH

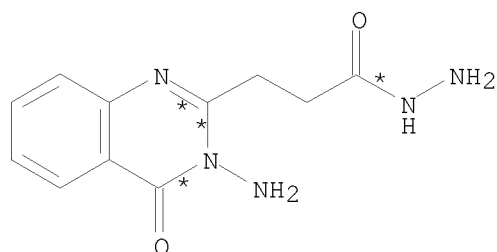
RX(30)      RCT    AI 120572-48-7  
              RGT    AG 302-01-2 N2H4  
              PRO    AL 120572-51-2  
              SOL    64-17-5 EtOH

RX(114) OF 137 COMPOSED OF RX(19), RX(22), RX(31)  
RX(114)    R    ==>    AL



R

3  
STEPS  
→



AL

RX(19) RCT R 120572-38-5  
RGT AG 302-01-2 N2H4  
PRO AF 84312-90-3  
SOL 64-17-5 EtOH

RX(22) RCT AF 84312-90-3  
RGT M 64-17-5 EtOH  
PRO AJ 120572-49-8  
CAT 7664-93-9 H2SO4  
SOL 64-17-5 EtOH

RX(31) RCT AJ 120572-49-8  
RGT AG 302-01-2 N2H4  
PRO AL 120572-51-2  
SOL 64-17-5 EtOH

L3 ANSWER 169 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 110:193170 CASREACT

TITLE: Incorporation of molecular nitrogen into organic compounds. 2. Novel lactam synthesis by use of a combination system of carbonylation and nitrogenation

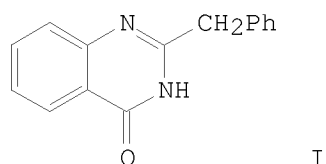
AUTHOR(S): Uozumi, Yasuhiro; Kawasaki, Naofumi; Mori, Eiko; Mori, Miwako; Shibasaki, Masakatsu

CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, 060, Japan

SOURCE: Journal of the American Chemical Society (1989),

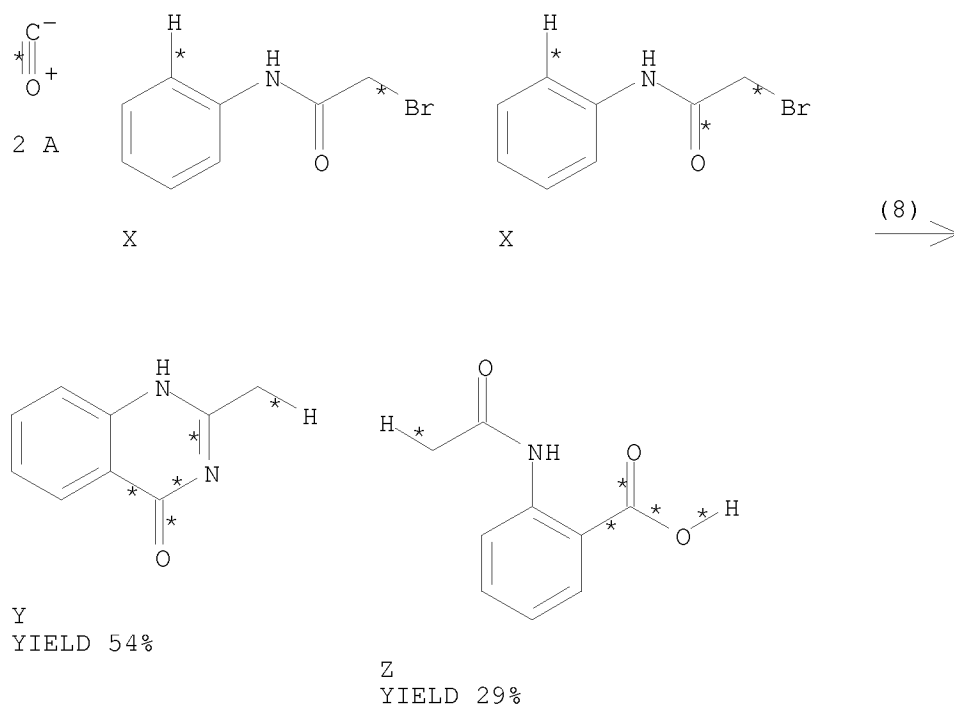
111(10), 3725-7  
 CODEN: JACSAT; ISSN: 0002-7863  
 Journal  
 English

DOCUMENT TYPE:  
 LANGUAGE:  
 GI



AB An amide unit was constructed from aryl halide and a TiNCO complex under atmospheric pressure of N and CO in the presence of a Pd catalyst. With this combination of carbonylation and nitrogenation, isoindolinone and quinazolinone derivs. were synthesized from o-halophenyl alkyl ketones in one step. The reaction proceeds through the oxidative addition of enol lactone, generated by Pd-catalyzed carbonylation to o-halophenyl alkyl ketone, to TiNCO complex. Glycosminine (I) was prepared in 40% yield by this method.

RX(8) OF 9      2 A + 2 X ==> Y + Z



RX(8)      RCT A 630-08-0

STAGE(1)

RGT E 7550-45-0 TiCl<sub>4</sub>, F 7439-95-4 Mg, G 7727-37-9 N<sub>2</sub>

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SOL 109-99-9 THF

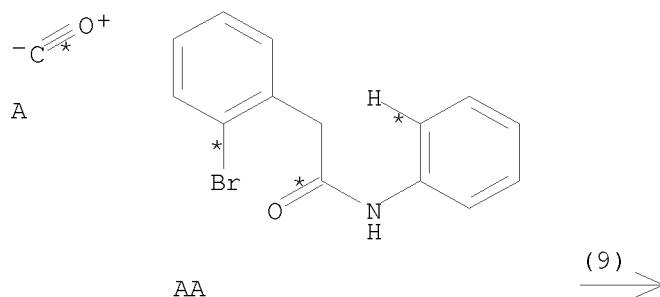
STAGE(2)

RCT X 5326-87-4  
RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
CAT 14221-01-3 Pd(PPh<sub>3</sub>)<sub>4</sub>  
SOL 872-50-4 NMEP

PRO Y 1769-24-0, Z 89-52-1

NTE NITROGEN ACTIVATED BY TITANIUM COMPLEX

RX(9) OF 9 A + AA ==> AB



AB  
YIELD 40%

RX(9) RCT A 630-08-0

STAGE(1)

RGT E 7550-45-0 TiCl<sub>4</sub>, F 7439-95-4 Mg, G 7727-37-9 N<sub>2</sub>  
SOL 109-99-9 THF

STAGE(2)

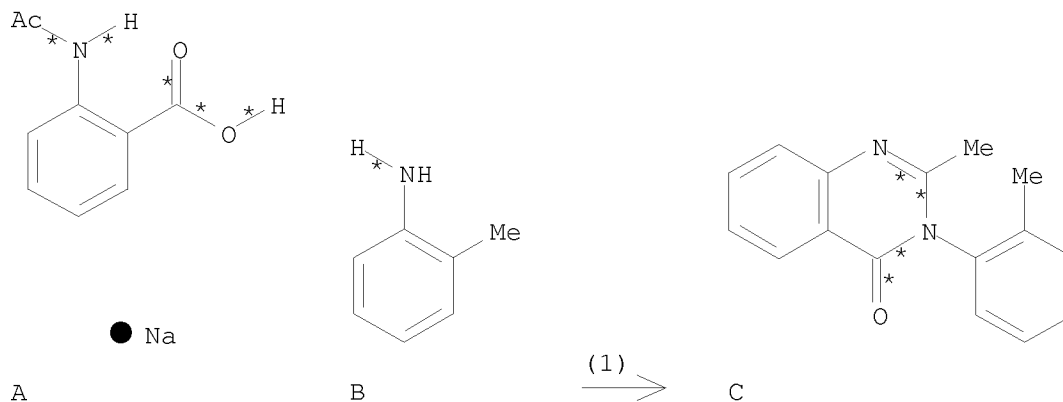
RCT AA 120230-90-2  
RGT H 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
CAT 14221-01-3 Pd(PPh<sub>3</sub>)<sub>4</sub>  
SOL 872-50-4 NMEP

PRO AB 4765-56-4

NTE NITROGEN ACTIVATED BY TITANIUM COMPLEX

L3 ANSWER 170 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 110:192758 CASREACT  
 TITLE: Synthesis of some new 2-styryl-3-o-tolyl-4-quinazolone  
 as compound of antifungal activity  
 AUTHOR(S): Rawat, Malti  
 CORPORATE SOURCE: Maharaja Coll., A. P. S. Univ., Rewa, India  
 SOURCE: Journal of the Institution of Chemists (India) (1988),  
 60(2), 58  
 CODEN: JOICA7; ISSN: 0020-3254  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Cyclocondensation of o-MeC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> with o-AcNHC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Na gave  
 2-methyl-3-o-tolyl-4-quinazolone, which reacted with PhCHO derivs. to give  
 the title compds. These compds. were tested for fungicidal activity  
 against Curvularia lunata and Fusarium oxysporum. The percentage of  
 inhibition was 22.5-40.3%.

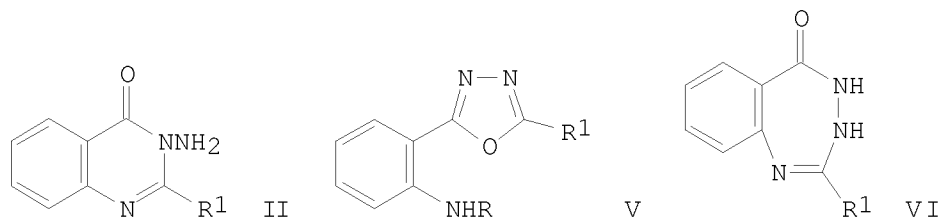
RX(1) OF 1 A + B ==> C



RX(1) RCT A 2870-60-2, B 95-53-4  
 RGT D 7719-12-2 PC13  
 PRO C 72-44-6

L3 ANSWER 171 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 110:173155 CASREACT  
 TITLE: Reaction of 2-aminobenzoylhydrazines with carboxylic  
 acids: formation of quinazolin-4(3H)-one,  
 1,3,4-oxadiazole and 1,3,4-benzotriazepin-5-one  
 derivatives  
 AUTHOR(S): Reddy, P. S. N.; Reddy, P. Pratap  
 CORPORATE SOURCE: Dep. Chem., Osmania Univ., Hyderabad, 500 007, India  
 SOURCE: Indian Journal of Chemistry, Section B: Organic  
 Chemistry Including Medicinal Chemistry (1988),  
 27B(8), 763-5  
 CODEN: IJSBDB; ISSN: 0376-4699

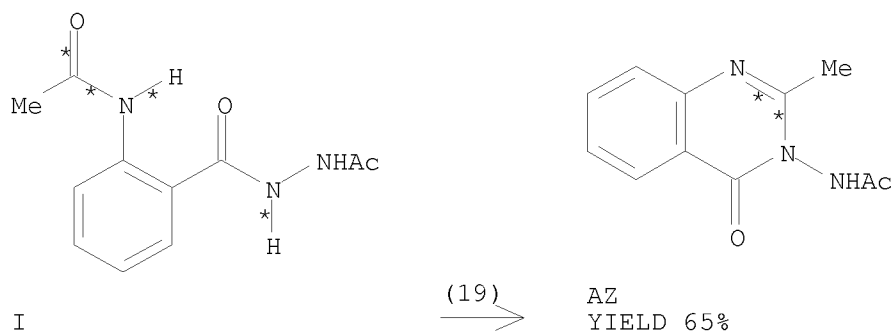
DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Reaction of 2-RNHC<sub>6</sub>H<sub>4</sub>CONHNH<sub>2</sub> (I; R = H) with R<sub>1</sub>CO<sub>2</sub>H [R<sub>1</sub> = H, Me, Et, Pr, Bu, Me(CH<sub>2</sub>)<sub>4</sub>] gave 2-R<sub>1</sub>CONHC<sub>6</sub>H<sub>4</sub>CONHNHCOR<sub>1</sub>, which cyclized with concentrate H<sub>2</sub>SO<sub>4</sub>

to give aminoquinazolinones II. R<sub>1</sub>CO<sub>2</sub>H (III; R<sub>1</sub> = Ph, substituted Ph, 2-furyl, 3-pyridyl) reacted with I (R = H) to give a mixture of 2-RNHC<sub>6</sub>H<sub>4</sub>CONHNHCOR<sub>1</sub> (IV), aryloxadiazoles V (R = H) and benzotriazepinones VI, while I (R = Me) reacted with III is given IV (R = Me) and V (R = Me).

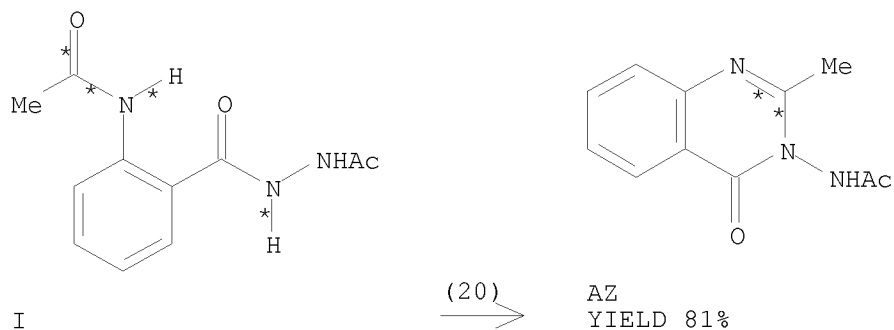
RX(19) OF 43      ...I    ==>    AZ



RX(19)      RCT    I 67571-08-8  
              PRO    AZ 6761-05-3  
              NTE    Thermal

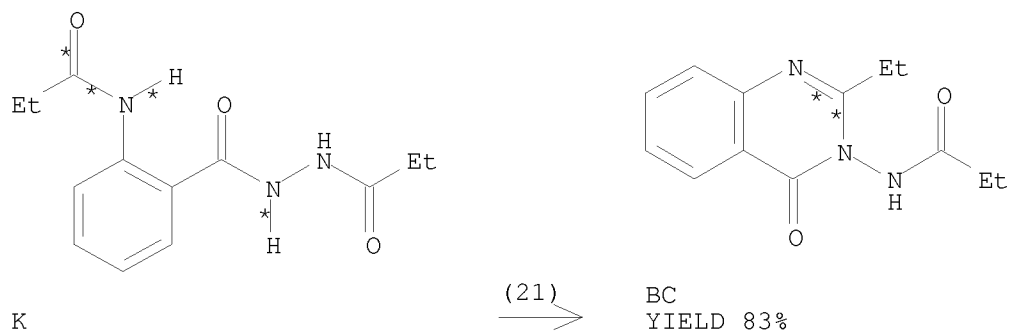
RX(20) OF 43      I    ==>    AZ

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RX(20)     RCT   I 67571-08-8  
             PRO   AZ 6761-05-3  
             CAT   104-15-4 TsOH  
             SOL   1330-20-7 Xylene  
             NTE   Thermal

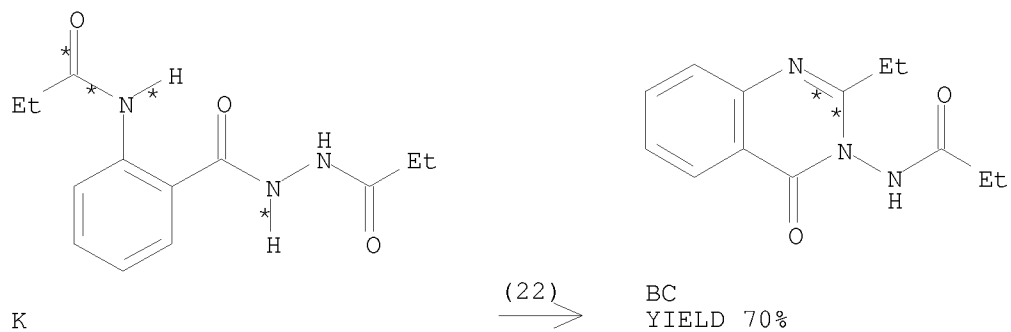
RX(21) OF 43     ...K   ==>   BC



RX(21)     RCT   K 67571-11-3  
             PRO   BC 6761-25-7  
             CAT   104-15-4 TsOH  
             SOL   1330-20-7 Xylene  
             NTE   Thermal

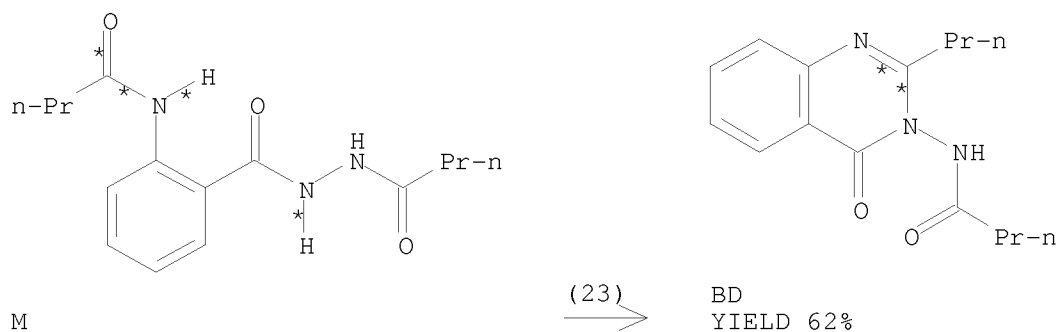
RX(22) OF 43     K   ==>   BC

10/ 562,112



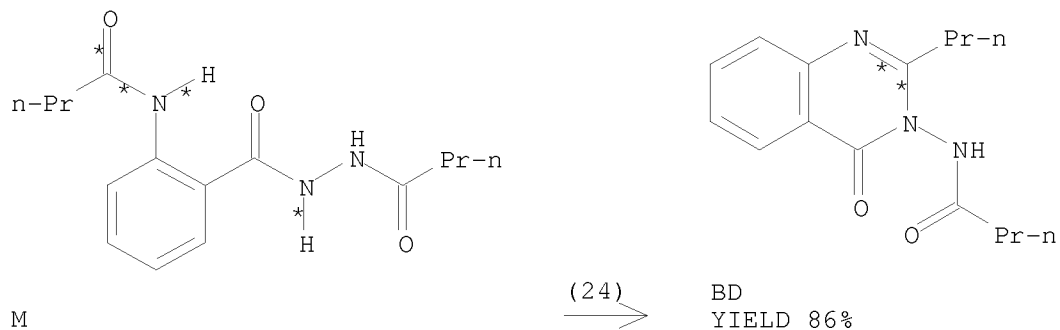
RX(22) RCT K 67571-11-3  
PRO BC 6761-25-7  
NTE Thermal

RX(23) OF 43 ...M ==> BD



RX(23) RCT M 120107-31-5  
PRO BD 120107-43-9  
NTE Thermal

RX(24) OF 43 M ==> BD

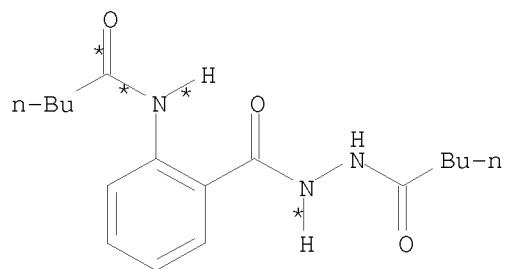




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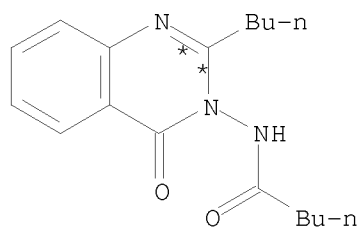
RX(24)      RCT    M 120107-31-5  
             PRO    BD 120107-43-9  
             CAT    104-15-4 TsOH  
             SOL    1330-20-7 Xylene  
             NTE    Thermal

RX(25) OF 43      ...O ==> BE



O

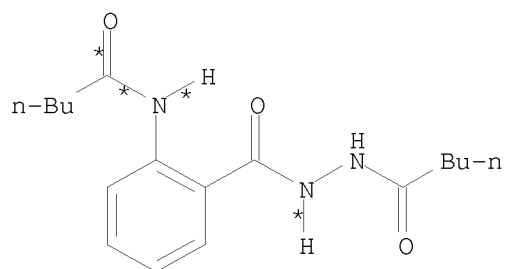
(25)  $\longrightarrow$



BE  
YIELD 77%

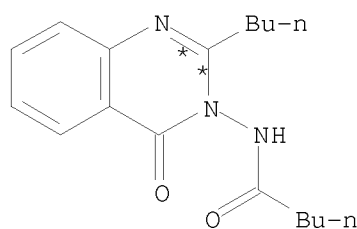
RX(25)      RCT    O 120107-32-6  
             PRO    BE 120107-44-0  
             CAT    104-15-4 TsOH  
             SOL    1330-20-7 Xylene  
             NTE    Thermal

RX(26) OF 43      O ==> BE



O

(26)  $\longrightarrow$

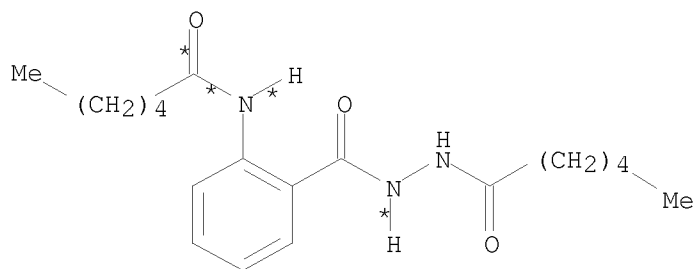


BE  
YIELD 68%

RX(26)      RCT    O 120107-32-6  
             PRO    BE 120107-44-0  
             NTE    Thermal

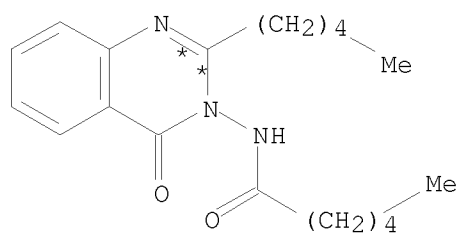
RX(27) OF 43      ...Q ==> BF

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Q

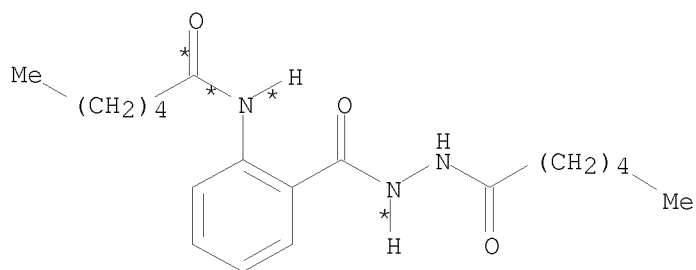
(27)  $\longrightarrow$



BF  
YIELD 65%

RX(27)      RCT    Q 120107-33-7  
              PRO    BF 120107-45-1  
              NTE    Thermal

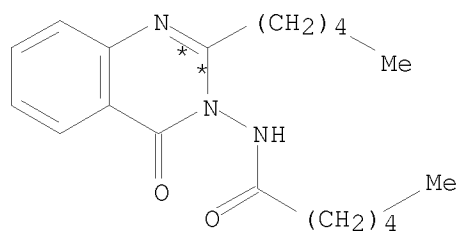
RX(28) OF 43      Q     $\implies$     BF



Q

(28)  $\longrightarrow$

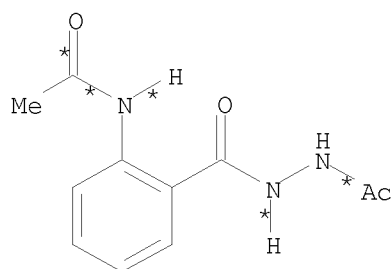
10/ 562,112



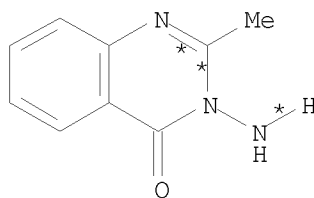
BF  
YIELD 80%

RX(28)      RCT    Q 120107-33-7  
              PRO    BF 120107-45-1  
              CAT    104-15-4 TsOH  
              SOL    1330-20-7 Xylene  
              NTE    Thermal

RX(29) OF 43      ...I    ==>    BG



I

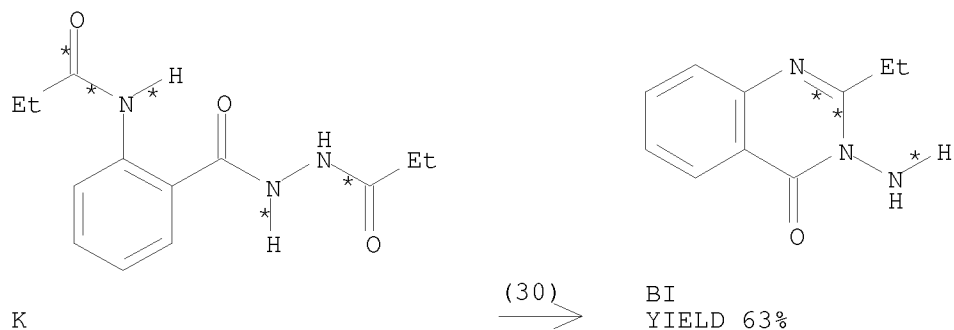


BG  
YIELD 58%

RX(29)      RCT    I 67571-08-8  
              RGT    BH 7664-93-9 H2SO4  
              PRO    BG 1898-06-2  
              SOL    7664-93-9 H2SO4

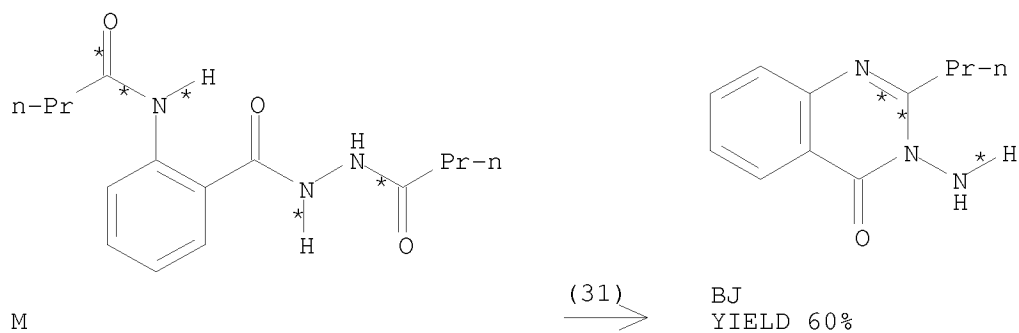
RX(30) OF 43      ...K    ==>    BI

10/ 562,112



RX(30) RCT K 67571-11-3  
RGT BH 7664-93-9 H2SO4  
PRO BI 50547-51-8  
SOL 7664-93-9 H2SO4

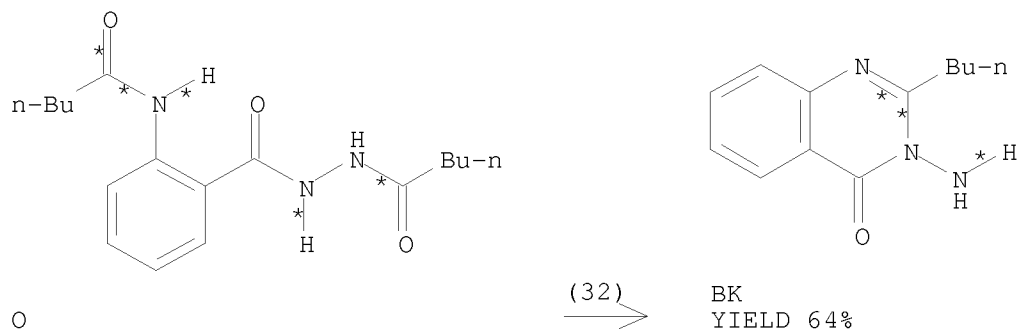
RX(31) OF 43 ...M ==> BJ



RX(31) RCT M 120107-31-5  
RGT BH 7664-93-9 H2SO4  
PRO BJ 84312-89-0  
SOL 7664-93-9 H2SO4

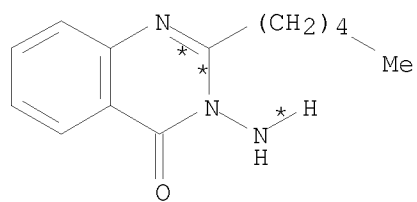
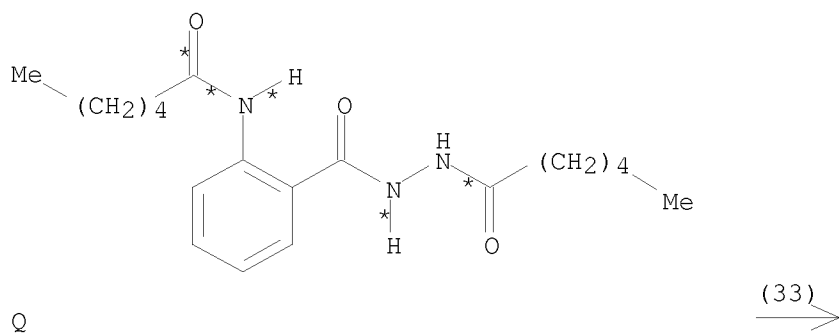
RX(32) OF 43 ...O ==> BK

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RX(32)      RCT   O 120107-32-6  
               RGT   BH 7664-93-9 H2SO4  
               PRO   BK 120107-46-2  
               SOL   7664-93-9 H2SO4

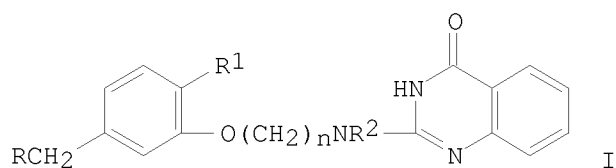
RX(33) OF 43      ...Q ==> BL



BL  
 YIELD 55%

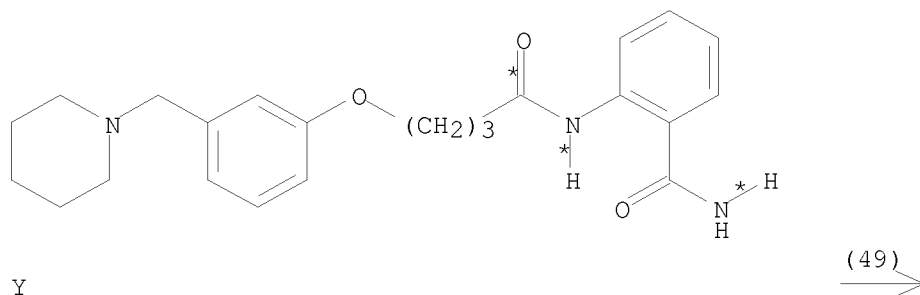
RX(33)      RCT   Q 120107-33-7  
               RGT   BH 7664-93-9 H2SO4  
               PRO   BL 120107-47-3  
               SOL   7664-93-9 H2SO4

L3 ANSWER 172 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 110:95158 CASREACT  
 TITLE: Synthesis and histamine H2-antagonist activity of  
 4-quinazolinone derivatives  
 AUTHOR(S): Ogawa, Nobuo; Yoshida, Toshihiko; Aratani, Takayuki;  
 Koshinaka, Eiichi; Kato, Hideo; Ito, Yasuo  
 CORPORATE SOURCE: Res. Lab., Hokuriku Seiyaku Co., Ltd., Inokuchi, 911,  
 Japan  
 SOURCE: Chemical & Pharmaceutical Bulletin (1988), 36(8),  
 2955-67  
 CODEN: CPBTAL; ISSN: 0009-2363  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

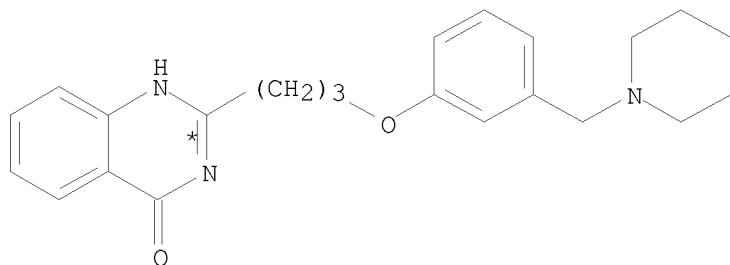


AB With the aim of developing new antiulcer agents, a series of 4-quinazolinone derivs. e.g., I (R = piperidino, pyrrolidino, morpholino, R1 = H, OMe, R2 = H, Me; n = 2, 3, 4) was synthesized and tested for histamine H2-antagonist activity and gastric antisecretory activity. Thus, 2-alkylamino-, 2-alkylthio-, and 2-alkyl-4-quinazolinones were prepared by the condensation of alkylamines with 2-chloro- or 2-methylthio-4-quinazolinones, the condensation of alkyl bromides with 2-mercapto-4-quinazolinones, and the condensation of alkylcarboxylic acids with anthranilamides, resp. Several of the 4-quinazolinone derivs. showed potent H2-antagonist activity, and one of them, I (R = piperidino, R1 = R2 = H, n = 3), showed the most potent antisecretory activity. The structure-activity relationships are discussed.

RX(49) OF 95 ...Y ==> DJ



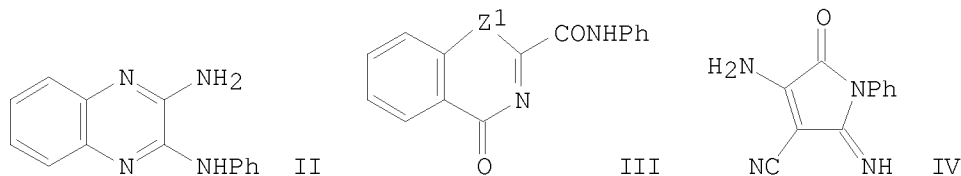
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DJ

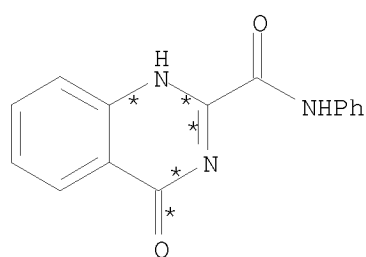
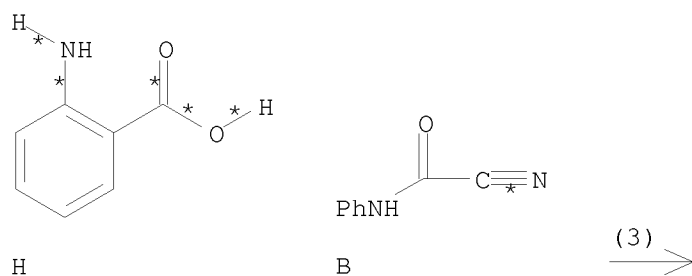
RX(49) RCT Y 119023-27-7  
RGT V 1310-73-2 NaOH  
PRO DJ 105189-23-9  
SOL 67-56-1 MeOH, 7732-18-5 Water

L3 ANSWER 173 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 110:38956 CASREACT  
TITLE: Nitriles in heterocyclic synthesis:  
1-cyanoformanilide as precursor for a variety of  
heterocyclic ring systems  
AUTHOR(S): Sherif, Sherif Mourad; Mohareb, Rafaat Milad;  
Elgemeie, Galal Eldin H.; Singh, Rajendra Prasad  
CORPORATE SOURCE: Fac. Sci., Cairo Univ., Giza, Egypt  
SOURCE: Heterocycles (1988), 27(7), 1579-83  
CODEN: HTCYAM; ISSN: 0385-5414  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB PhNHCOCN (I) was converted to quinoxaline derivative II and other heterocycles III (Z1 = O, NH). I was treated with o-phenylenediamine in DMF containing piperidine to give II. III (Z1 = O) was prepared from I, salicylic acid, and Et3N in EtOH. Pyrrolinone IV was obtained from I and CH2(CN)2.

RX(3) OF 10 H + B ==> I

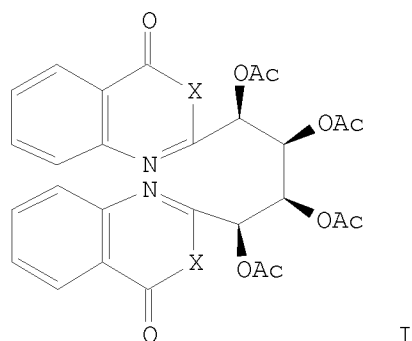


I

RX(3)      RCT    H 118-92-3, B 6784-22-1  
              PRO    I 118372-87-5  
              CAT    121-44-8 Et3N  
              SOL    64-17-5 EtOH

L3    ANSWER 174 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER:      109:231445    CASREACT  
 TITLE:                    Heterocycles from carbohydrate precursors. Part 46.  
                               A novel approach for the synthesis of C-nucleoside  
                               analogs by constructing benzoxazine rings linked to a  
                               carbohydrate moiety  
 AUTHOR(S):                El Ashry, El Sayed H.; Rashed, Nagwa; Mousaad, Ahmed  
 CORPORATE SOURCE:        Fac. Sci., Alexandria Univ., Alexandria, Egypt  
 SOURCE:                    Journal of Carbohydrate Chemistry (1987), 6(4),  
                                   599-607  
                                   CODEN: JCACDM; ISSN: 0732-8303  
 DOCUMENT TYPE:            Journal  
 LANGUAGE:                 English  
 GI

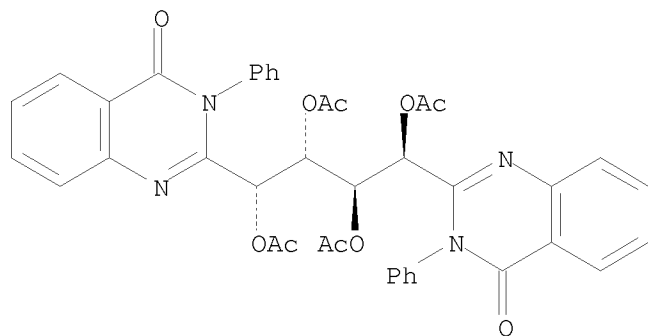
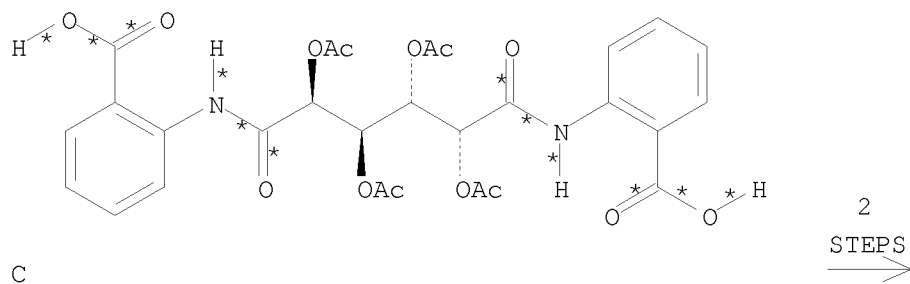




AB Dehydrative cyclization of the condensation product of 2,3,4,5-tetra-O-acetylgalactaryl chloride with anthranilic acid gave 1,2,3,4-tetra-O-acetyl-1,4-bis(4H-benzoxazin-4-one-2-yl)-galacto-tetritol (I, X = O). Its reaction with PhNH<sub>2</sub> in the presence of PCl<sub>3</sub> afforded 1,4-bis(3-phenylquinazolin-4-one-2-yl)-1,2,3,4-tetra-O-acetyl-galacto-tetritol (I, X = NPh).

RX(9) OF 11 COMPOSED OF RX(2), RX(6)

RX(9) C ==> K



YIELD 77%

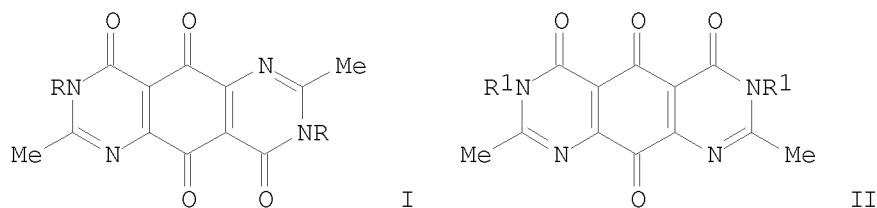
RX(2) RCT C 82185-59-9

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RGT G 108-24-7 Ac2O  
PRO F 82185-60-2

RX(6) RCT F 82185-60-2  
RGT L 7719-12-2 PC13  
PRO K 117641-26-6  
SOL 108-88-3 PhMe

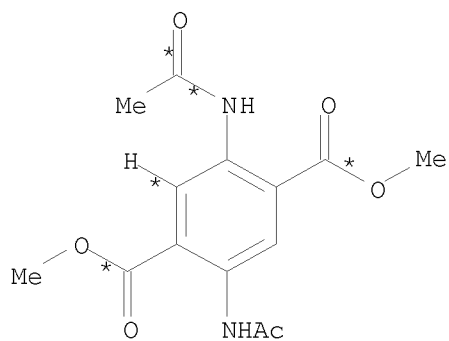
L3 ANSWER 175 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 109:128947 CASREACT  
TITLE: Synthesis and electrochemistry of  
pyrimidoquinazoline-5,10-diones. Design of  
hydrolytically stable high potential quinones and new  
reductive alkylation systems  
AUTHOR(S): Skibo, Edward B.; Gilchrist, James H.  
CORPORATE SOURCE: Dep. Chem., Arizona State Univ., Tempe, AZ,  
85287-1604, USA  
SOURCE: Journal of Organic Chemistry (1988), 53(18), 4209-18  
CODEN: JOCEAH; ISSN: 0022-3263  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB The synthesis of pyrimido[4,5-g]quinazoline-5,10-diones I (R = H, Me) and pyrimido[5,4-g]quinazoline-5,10-diones II (R1 = H, Me) was carried out in conjunction with the design of both hydrolytically stable high potential quinones and new purine-like reductive alkylating agents. I and II consist of a benzoquinone ring bearing two fused pyrimidinone rings. The fused pyrimidinone rings serve to protect I and II from hydrolysis as well as to raise quinone redox potentials by stabilizing the hydroquinones with internal H bonds (65 mV increase per H bond). Synthesis of I and II involved pyrimidinone ring annulation to a 2,5-diamino-3-nitroterephthalic acid derivative and to a 2,4-diamino-1,5-dicarboxy-3-nitrobenzene derivative, resp. The synthetic studies provided insights into the electronic effects of nitro and amino groups on the annulation process.

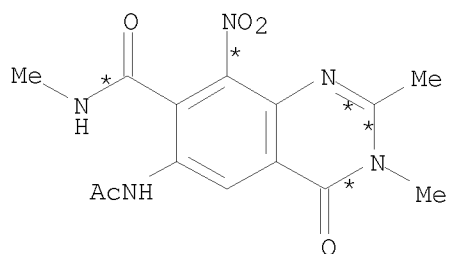
RX(36) OF 141 COMPOSED OF RX(7), RX(8)  
RX(36) P ==> U

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P

2  
STEPS  
→



U

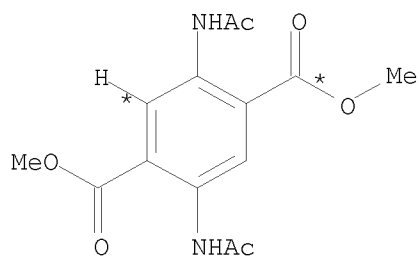
YIELD 51%

RX(7) RCT P 115705-52-7  
RGT T 50-00-0 HCHO, J 7697-37-2 HNO3  
PRO S 115705-53-8  
SOL 7697-37-2 HNO3

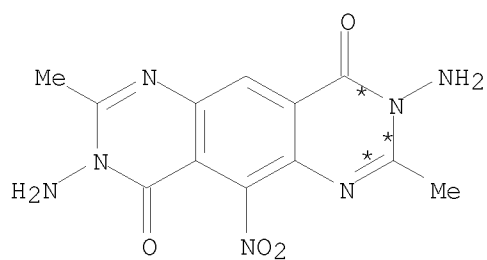
RX(8) RCT S 115705-53-8  
RGT V 74-89-5 MeNH2  
PRO U 115705-55-0  
SOL 68-12-2 DMF, 67-56-1 MeOH

RX(37) OF 141 COMPOSED OF RX(7), RX(10)  
RX(37) P + Y ==> Z

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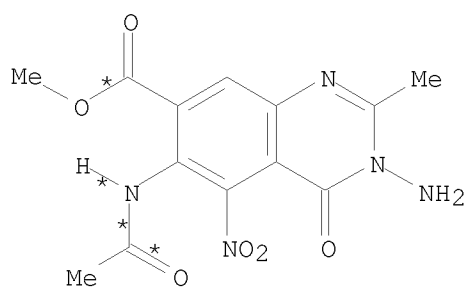


P



Y

2  
STEPS  
→

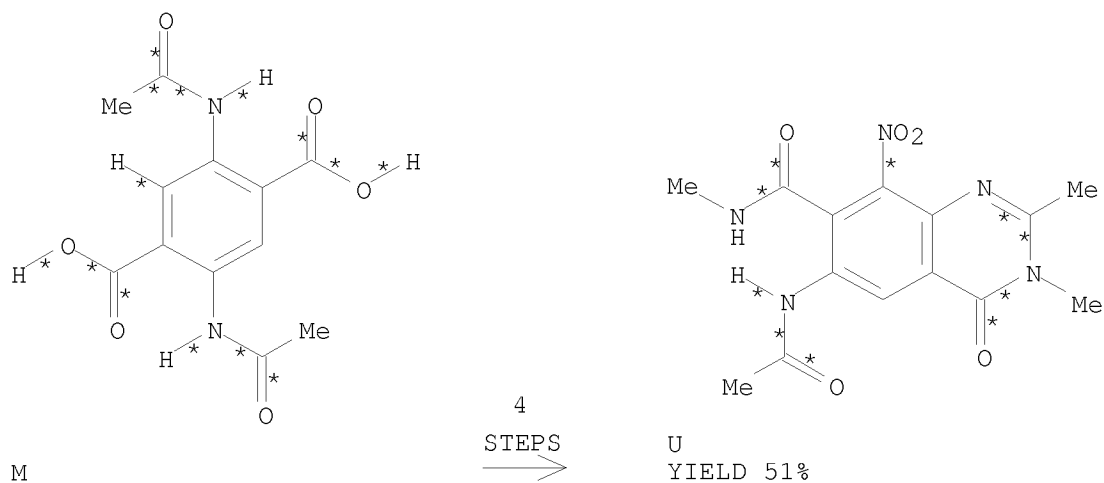


Z  
YIELD 69%

RX(7)      RCT    P 115705-52-7  
              RGT    T 50-00-0 HCHO, J 7697-37-2 HNO3  
              PRO    S 115705-53-8  
              SOL    7697-37-2 HNO3

RX(10)     RCT    S 115705-53-8, Y 115705-56-1  
              RGT    AA 302-01-2 N2H4  
              PRO    Z 115705-54-9  
              SOL    67-56-1 MeOH

RX(67) OF 141 COMPOSED OF RX(5), RX(6), RX(7), RX(8)  
RX(67)      M    ==>    U



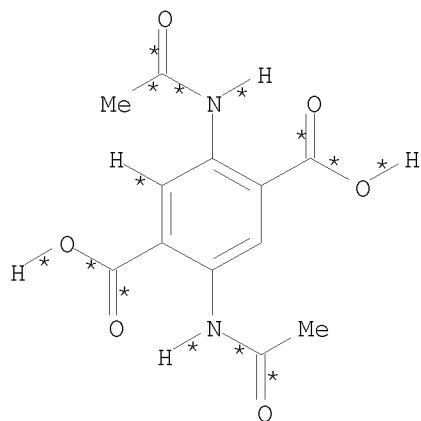
RX(5) RCT M 115705-51-6  
 RGT L 108-24-7 Ac2O  
 PRO N 22438-03-5  
 SOL 64-19-7 AcOH, 108-24-7 Ac2O

RX(6) RCT N 22438-03-5  
 RGT Q 124-41-4 NaOMe  
 PRO P 115705-52-7  
 SOL 67-56-1 MeOH

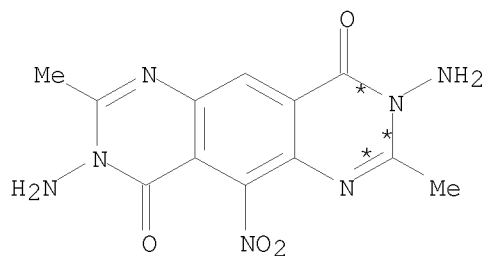
RX(7) RCT P 115705-52-7  
 RGT T 50-00-0 HCHO, J 7697-37-2 HNO3  
 PRO S 115705-53-8  
 SOL 7697-37-2 HNO3

RX(8) RCT S 115705-53-8  
 RGT V 74-89-5 MeNH2  
 PRO U 115705-55-0  
 SOL 68-12-2 DMF, 67-56-1 MeOH

RX(68) OF 141 COMPOSED OF RX(5), RX(6), RX(7), RX(10)  
 RX(68) M + Y ==> Z

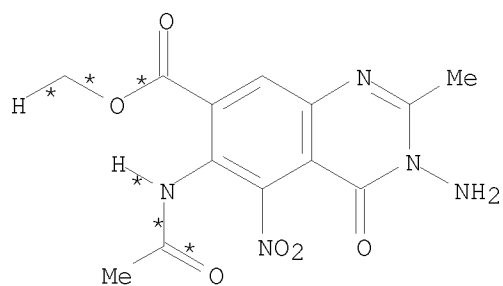


M



Y

4  
STEPS  
→



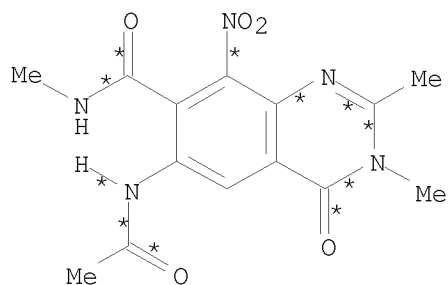
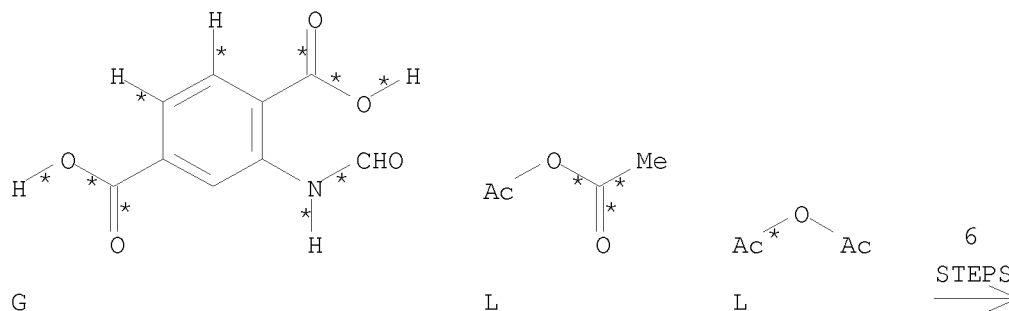
Z  
YIELD 69%

RX(5)	RCT	M 115705-51-6
	RGT	L 108-24-7 Ac2O
	PRO	N 22438-03-5
	SOL	64-19-7 AcOH, 108-24-7 Ac2O
RX(6)	RCT	N 22438-03-5
	RGT	Q 124-41-4 NaOMe
	PRO	P 115705-52-7
	SOL	67-56-1 MeOH
RX(7)	RCT	P 115705-52-7
	RGT	T 50-00-0 HCHO, J 7697-37-2 HNO3
	PRO	S 115705-53-8
	SOL	7697-37-2 HNO3
RX(10)	RCT	S 115705-53-8, Y 115705-56-1
	RGT	AA 302-01-2 N2H4
	PRO	Z 115705-54-9
	SOL	67-56-1 MeOH

RX(105) OF 141 COMPOSED OF RX(3), RX(4), RX(5), RX(6), RX(7), RX(8)

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RX(105) G + 2 L ==> U



U  
YIELD 51%

RX(3) RCT G 115705-49-2  
RGT J 7697-37-2 HNO3, K 7664-93-9 H2SO4  
PRO I 115705-50-5  
SOL 7697-37-2 HNO3, 7664-93-9 H2SO4

RX(4) RCT I 115705-50-5, L 108-24-7  
RGT C 1333-74-0 H2, D 1310-58-3 KOH  
PRO M 115705-51-6  
CAT 7440-05-3 Pd  
SOL 7732-18-5 Water

RX(5) RCT M 115705-51-6  
RGT L 108-24-7 Ac2O  
PRO N 22438-03-5  
SOL 64-19-7 AcOH, 108-24-7 Ac2O

RX(6) RCT N 22438-03-5  
RGT Q 124-41-4 NaOMe  
PRO P 115705-52-7  
SOL 67-56-1 MeOH

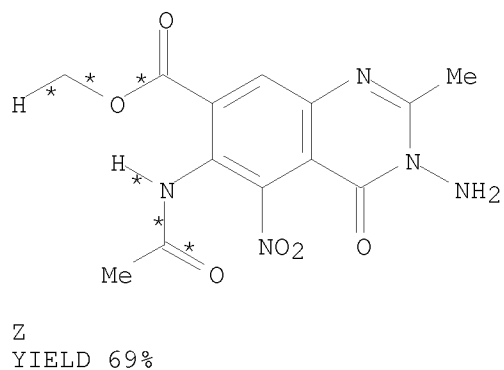
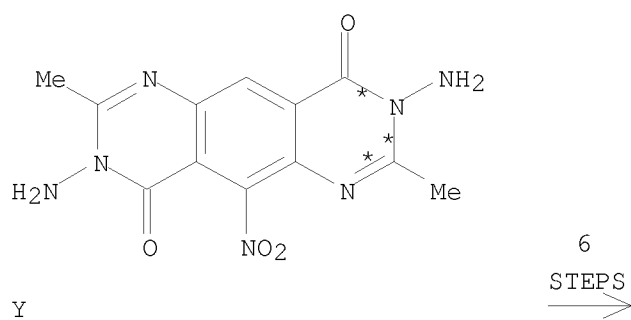
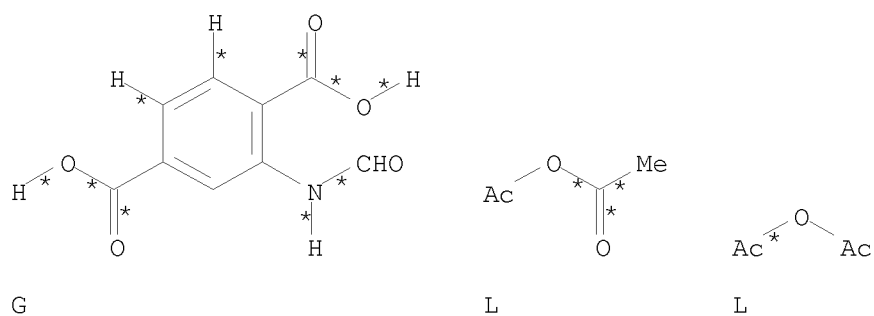
RX(7) RCT P 115705-52-7  
RGT T 50-00-0 HCHO, J 7697-37-2 HNO3  
PRO S 115705-53-8  
SOL 7697-37-2 HNO3

RX(8) RCT S 115705-53-8

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RGT V 74-89-5 MeNH2  
PRO U 115705-55-0  
SOL 68-12-2 DMF, 67-56-1 MeOH

RX(106) OF 141 COMPOSED OF RX(3), RX(4), RX(5), RX(6), RX(7), RX(10)  
RX(106) G + 2 L + Y ==> Z



RX(3) RCT G 115705-49-2  
RGT J 7697-37-2 HNO3, K 7664-93-9 H2SO4  
PRO I 115705-50-5  
SOL 7697-37-2 HNO3, 7664-93-9 H2SO4



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RX(4) RCT I 115705-50-5, L 108-24-7  
RGT C 1333-74-0 H2, D 1310-58-3 KOH  
PRO M 115705-51-6  
CAT 7440-05-3 Pd  
SOL 7732-18-5 Water

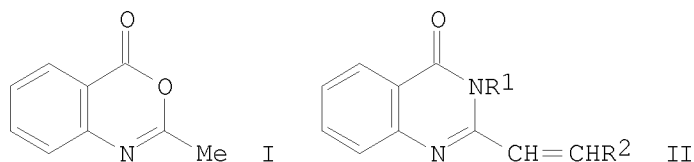
RX(5) RCT M 115705-51-6  
RGT L 108-24-7 Ac2O  
PRO N 22438-03-5  
SOL 64-19-7 AcOH, 108-24-7 Ac2O

RX(6) RCT N 22438-03-5  
RGT Q 124-41-4 NaOMe  
PRO P 115705-52-7  
SOL 67-56-1 MeOH

RX(7) RCT P 115705-52-7  
RGT T 50-00-0 HCHO, J 7697-37-2 HNO3  
PRO S 115705-53-8  
SOL 7697-37-2 HNO3

RX(10) RCT S 115705-53-8, Y 115705-56-1  
RGT AA 302-01-2 N2H4  
PRO Z 115705-54-9  
SOL 67-56-1 MeOH

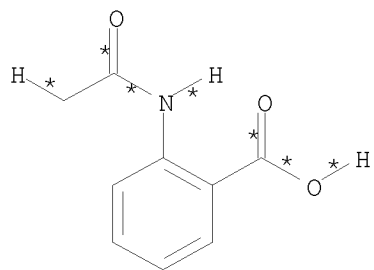
L3 ANSWER 176 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 109:92923 CASREACT  
TITLE: One-pot conversion of 2-methyl-3,1-benzoxazin-4-one  
into 3-substituted-2-styrylquinazolin-4-ones  
AUTHOR(S): Jain, Archana; Mukerjee, Arya K.  
CORPORATE SOURCE: Fac. Sci., Banaras Hindu Univ., Varanasi, 221 005,  
India  
SOURCE: Journal of the Indian Chemical Society (1987), 64(10),  
645-6  
CODEN: JICSAH; ISSN: 0019-4522  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



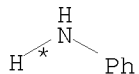
AB Benzoxazinone I was treated with R1NH2 (R1 = Ph, ClC6H4, anisyl, HO2CC6H4) and R2CHO [R2 = Ph, HOC6H4, HO(MeO)C6H3] to give styrylquinazolinones II. The treatment of 2-AcNHC6H4CO2H with tosyl chloride and Et3N gave I.

RX(8) OF 13 COMPOSED OF RX(1), RX(2)

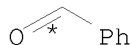
10/ 562,112

$$\text{RX (8)} \quad \text{A} + \text{F} + \text{G} \implies \text{H}$$


A

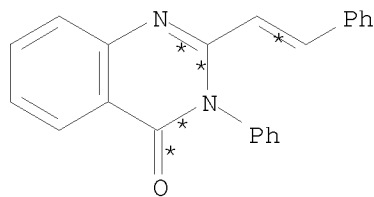


F



G

2  
STEPS  
→



H

RX(1)	RCT	A 89-52-1	
	RGT	C 98-59-9	TsCl, D 121-44-8 Et3N
	PRO	B 525-76-8	
	SOL	71-43-2	Benzene

RX(2) RCT B 525-76-8, F 62-53-3

STAGE (1)  
SOL 64-19-7 AcOH

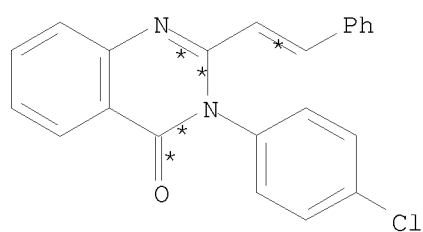
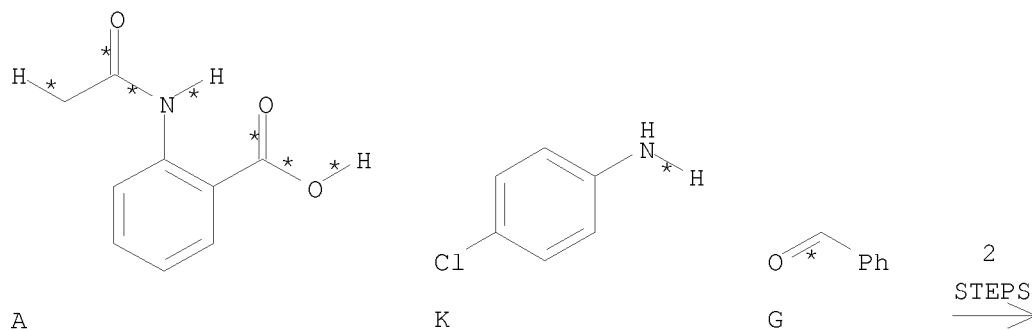
```
STAGE(2)
      RCT   G 100-52-7
      CAT   127-09-3 AcONa
```

PRO H 77143-60-3

RX(9) OF 13 COMPOSED OF RX(1), RX(3)

$$\text{RX (9)} \quad \text{A} + \text{K} + \text{G} \implies \text{L}$$

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RX(1) RCT A 89-52-1  
RGT C 98-59-9 TsCl, D 121-44-8 Et3N  
PRO B 525-76-8  
SOL 71-43-2 Benzene

RX(3) RCT B 525-76-8, K 106-47-8

STAGE(1)  
SOL 64-19-7 AcOH

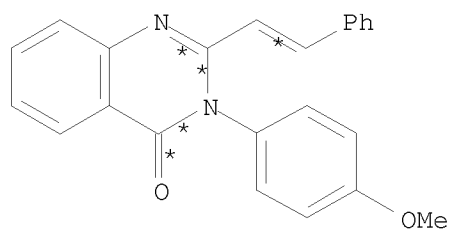
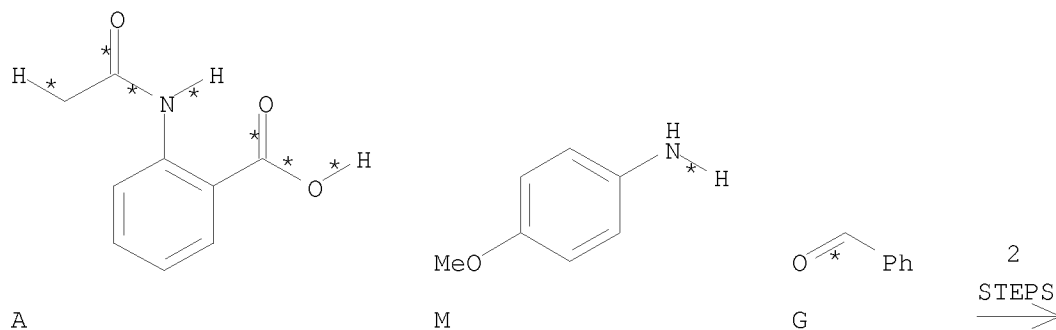
STAGE(2)  
RCT G 100-52-7  
CAT 127-09-3 AcONa

PRO L 115781-69-6

RX(10) OF 13 COMPOSED OF RX(1), RX(4)

RX(10) A + M + G ==> N

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RX(1) RCT A 89-52-1  
RGT C 98-59-9 TsCl, D 121-44-8 Et3N  
PRO B 525-76-8  
SOL 71-43-2 Benzene

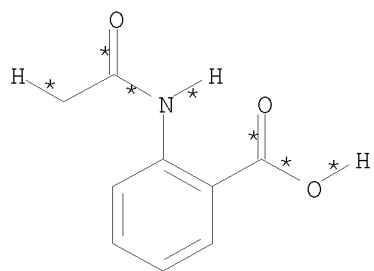
RX(4) RCT B 525-76-8, M 104-94-9

STAGE(1)  
SOL 64-19-7 AcOH

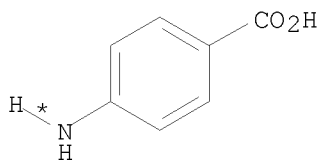
STAGE(2)  
RCT G 100-52-7  
CAT 127-09-3 AcONa

PRO N 115781-70-9

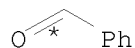
RX(11) OF 13 COMPOSED OF RX(1), RX(5)  
RX(11) A + O + G ==> P



A

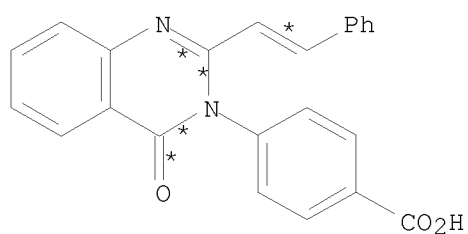


O



G

2  
STEPS  
→



P

RX(1) RCT A 89-52-1  
RGT C 98-59-9 TsCl, D 121-44-8 Et3N  
PRO B 525-76-8  
SOL 71-43-2 Benzene

RX(5) RCT B 525-76-8, O 150-13-0

STAGE(1)  
SOL 64-19-7 AcOH

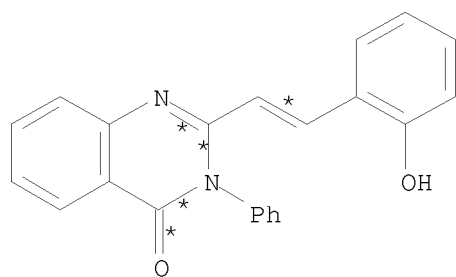
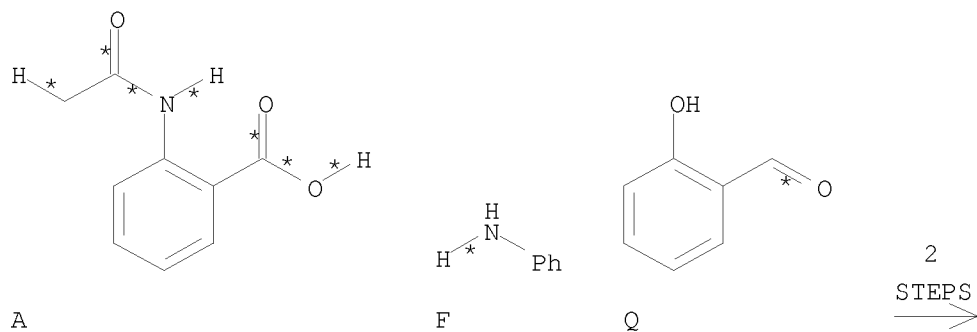
STAGE(2)  
RCT G 100-52-7  
CAT 127-09-3 AcONa

PRO P 37856-33-0

RX(12) OF 13 COMPOSED OF RX(1), RX(6)

RX(12) A + F + Q ==> R

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R

RX(1) RCT A 89-52-1  
 RGT C 98-59-9 TsCl, D 121-44-8 Et3N  
 PRO B 525-76-8  
 SOL 71-43-2 Benzene

RX(6) RCT B 525-76-8, F 62-53-3

STAGE(1)  
 SOL 64-19-7 AcOH

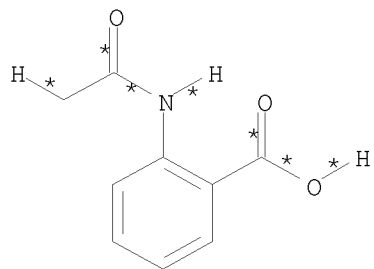
STAGE(2)  
 RCT Q 90-02-8  
 CAT 127-09-3 AcONa

PRO R 77815-33-9

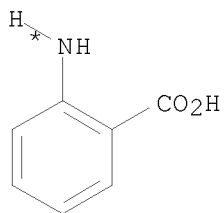
RX(13) OF 13 COMPOSED OF RX(1), RX(7)

RX(13) A + S + T ==> U

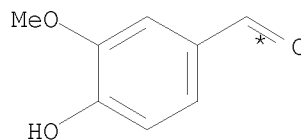
10/ 562,112



A

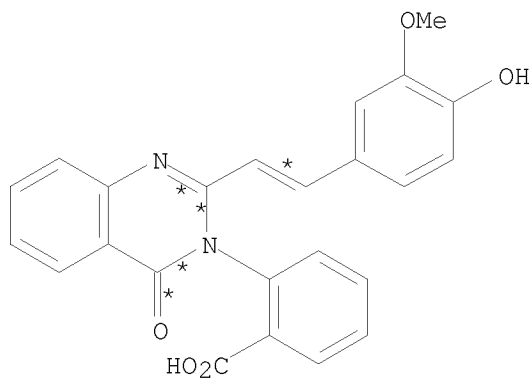


S



T

2  
STEPS  
→



U

RX(1)      RCT    A 89-52-1  
             RGT    C 98-59-9 TsCl, D 121-44-8 Et3N  
             PRO    B 525-76-8  
             SOL    71-43-2 Benzene

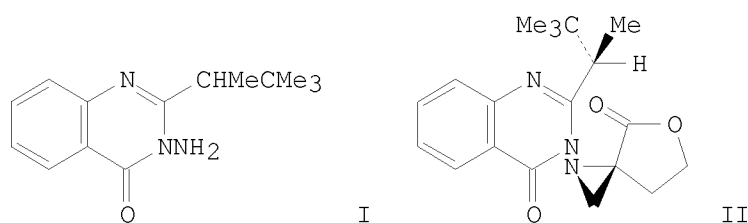
RX(7)      RCT    B 525-76-8, S 118-92-3

STAGE(1)  
SOL    64-19-7 AcOH

STAGE(2)  
RCT    T 121-33-5  
CAT    127-09-3 AcONa

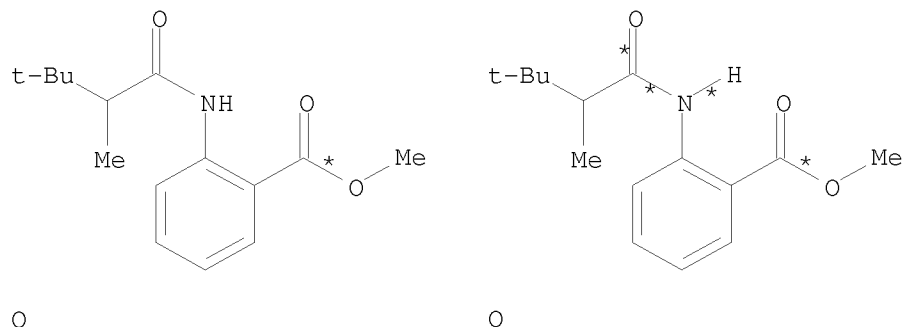
PRO    U 72743-31-8

L3 ANSWER 177 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 109:92918 CASREACT  
 TITLE: Asymmetric induction in addition of N-nitrenes to alkenes. Oxidation of 3-amino-2-(1,2,2-trimethylpropyl)quinazolin-4(3H)-one in the presence of  $\alpha$ -methylene- $\gamma$ -butyrolactone: conformation analysis of the aziridines formed and comparison with alkanoylated cyclopropylamines  
 AUTHOR(S): Atkinson, Robert S.; Tughan, Gary  
 CORPORATE SOURCE: Dep. Chem., Univ. Leicester, Leicester, LE1 7RH, UK  
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (12), 2797-802  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



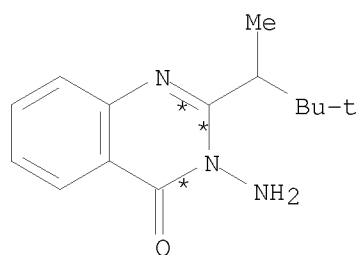
AB Oxidation of the title N-aminoquinazolinone (I) in the presence of  $\alpha$ -methylene- $\gamma$ -butyrolactone yields the spiroaziridines II with virtually no asym. induction. The same oxidation carried out in the presence of 3.4 mol. equivalent of CF<sub>3</sub>CO<sub>2</sub>H yielded only a single stereoisomer. The mol. structure reveals an unexpected orientation around the N-N bound by comparison with other hydrazines. The NMR spectra of the isomers of II show that both aziridines exist in solution as single invertomers at nitrogen: one isomer shows the presence of both rotamers around the N-N bond, but only one rotamer is evident for the other.

RX(5) OF 24 2 O ==> A + P...

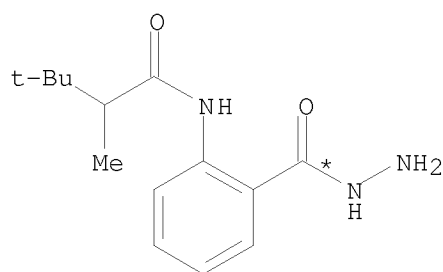




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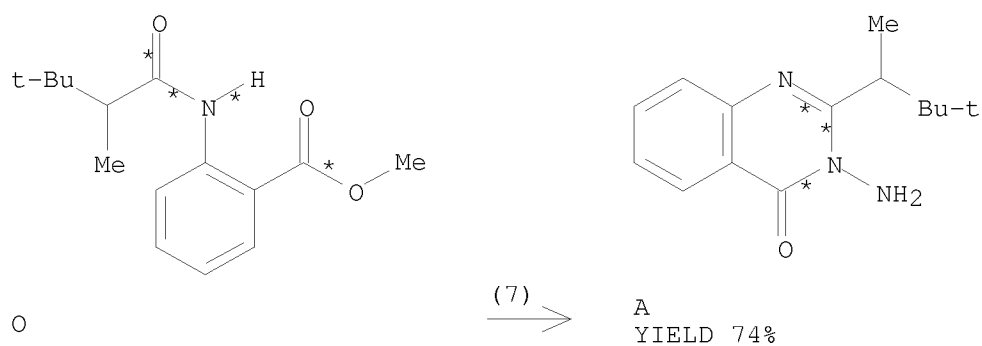
A  
YIELD 24%



P  
YIELD 55%

RX(5)      RCT    O 115875-69-9  
             RGT    Q 302-01-2 N2H4  
             PRO    A 116065-10-2, P 115855-35-1  
             SOL    64-17-5 EtOH

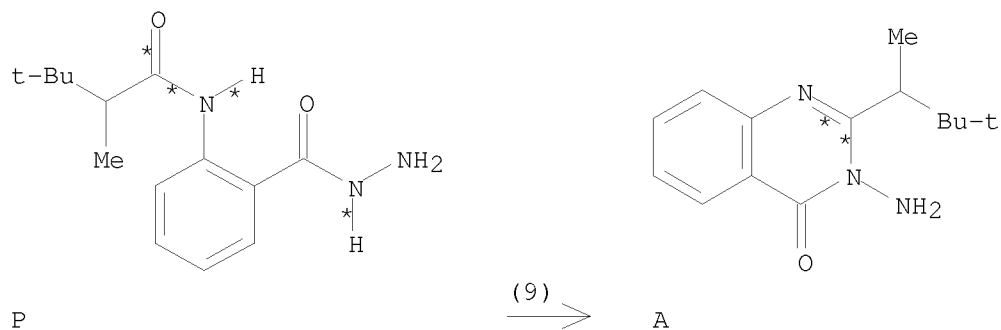
RX(7) OF 24      O    ==>    A...



RX(7)      RCT    O 115875-69-9  
             RGT    Q 302-01-2 N2H4  
             PRO    A 116065-10-2  
             SOL    64-17-5 EtOH

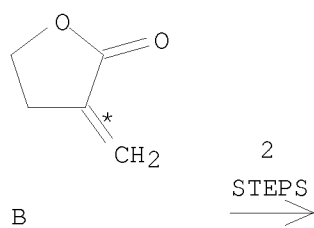
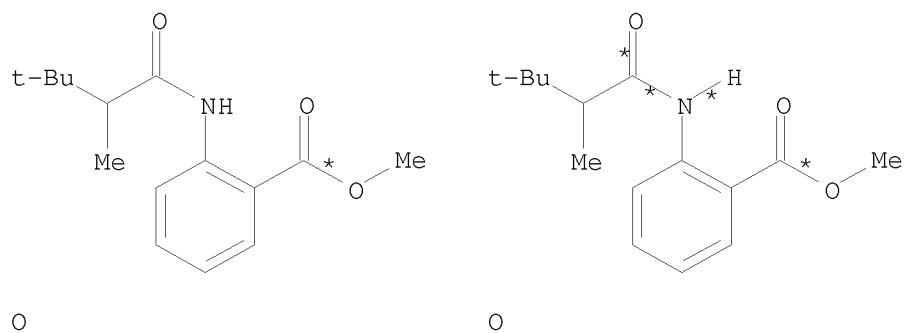
RX(9) OF 24      ...P    ==>    A...

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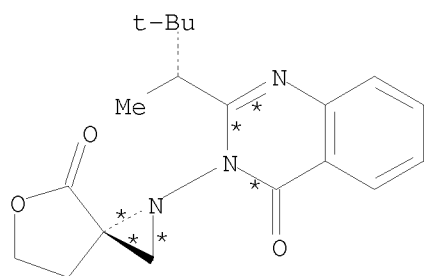


RX(9) RCT P 115855-35-1  
 PRO A 116065-10-2  
 SOL 64-17-5 EtOH

RX(11) OF 24 COMPOSED OF RX(5), RX(1)  
 RX(11) 2 O + B ==> C



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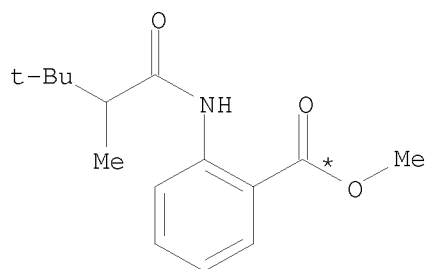


C  
YIELD 72%

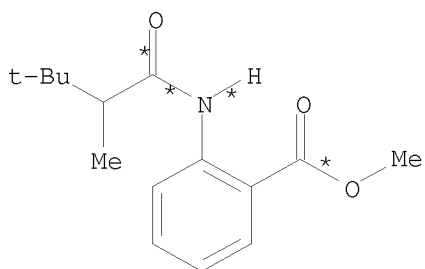
RX(5)      RCT    O 115875-69-9  
              RGT    Q 302-01-2 N2H4  
              PRO    A 116065-10-2, P 115855-35-1  
              SOL    64-17-5 EtOH

RX(1)      RCT    A 116065-10-2, B 547-65-9  
              RGT    D 546-67-8 Pb(OAc)4, E 76-05-1 F3CCO2H  
              PRO    C 105983-10-6  
              SOL    75-09-2 CH2Cl2

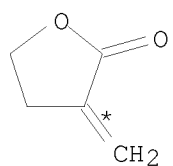
RX(12) OF 24 COMPOSED OF RX(5), RX(2)  
RX(12)      3 O + 2 B ==> C + G



0



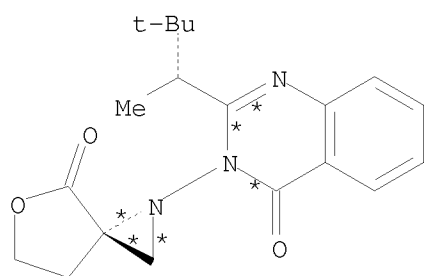
2 0



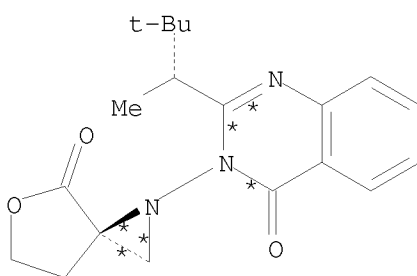
2 B

2  
STEPS  
→

10/ 562,112



C



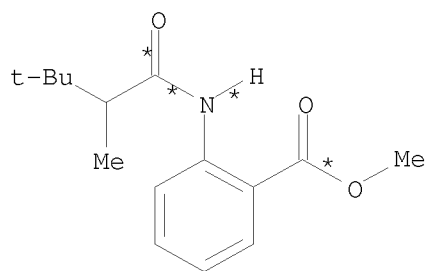
G

RX(5)      RCT    O 115875-69-9  
              RGT    Q 302-01-2 N2H4  
              PRO    A 116065-10-2, P 115855-35-1  
              SOL    64-17-5 EtOH

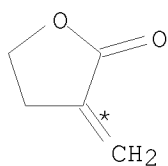
RX(2)      RCT    A 116065-10-2, B 547-65-9  
              RGT    D 546-67-8 Pb(OAc)4  
              PRO    C 105983-10-6, G 105983-09-3  
              SOL    75-09-2 CH2Cl2

RX(13) OF 24 COMPOSED OF RX(7), RX(1)

RX(13)      O + B ==> C

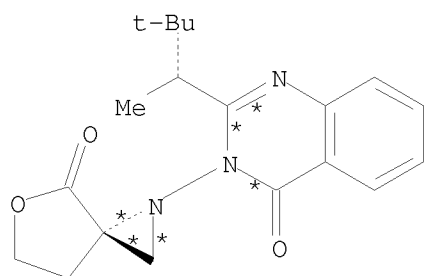


O



B

2  
 STEPS  
 →



C

YIELD 72%

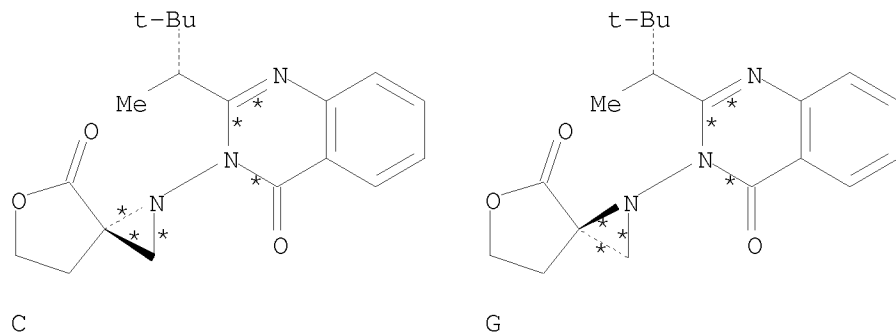
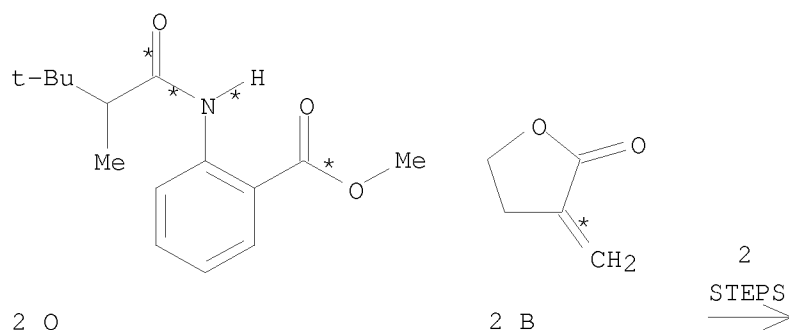
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RX(7)      RCT   O 115875-69-9  
             RGT   Q 302-01-2 N2H4  
             PRO   A 116065-10-2  
             SOL   64-17-5 EtOH

RX(1)      RCT   A 116065-10-2, B 547-65-9  
             RGT   D 546-67-8 Pb(OAc)4, E 76-05-1 F3CCO2H  
             PRO   C 105983-10-6  
             SOL   75-09-2 CH2Cl2

RX(14) OF 24 COMPOSED OF RX(7), RX(2)

RX(14)      2 O + 2 B ==> C + G



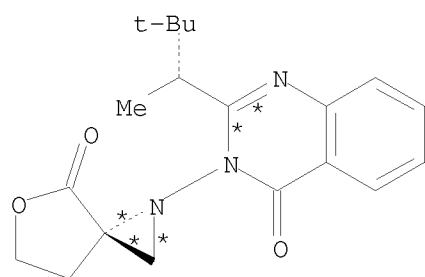
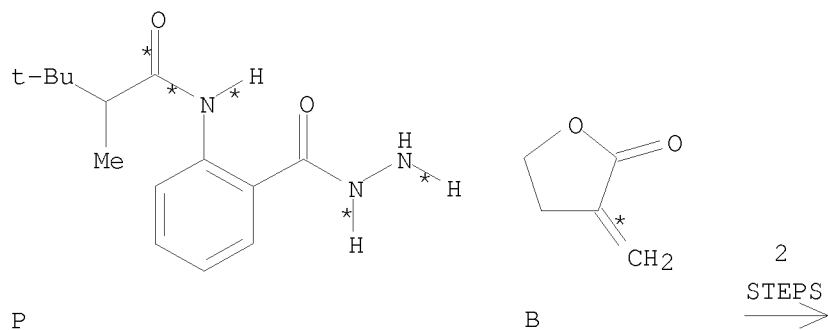
RX(7)      RCT   O 115875-69-9  
             RGT   Q 302-01-2 N2H4  
             PRO   A 116065-10-2  
             SOL   64-17-5 EtOH

RX(2)      RCT   A 116065-10-2, B 547-65-9  
             RGT   D 546-67-8 Pb(OAc)4  
             PRO   C 105983-10-6, G 105983-09-3  
             SOL   75-09-2 CH2Cl2

RX(15) OF 24 COMPOSED OF RX(9), RX(1)

RX(15)      P + B ==> C

10/ 562,112



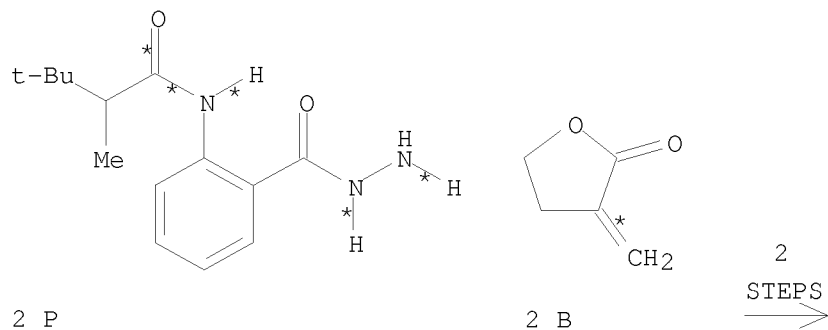
YIELD 72%

RX(9) RCT P 115855-35-1  
PRO A 116065-10-2  
SOL 64-17-5 EtOH

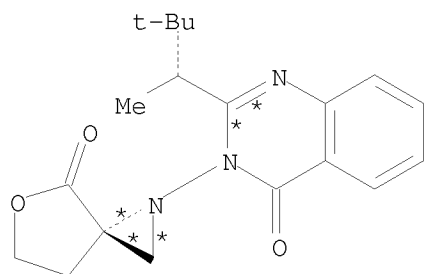
RX(1) RCT A 116065-10-2, B 547-65-9  
RGT D 546-67-8 Pb(OAc)<sub>4</sub>, E 76-05-1 F<sub>3</sub>CCO<sub>2</sub>H  
PRO C 105983-10-6  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(16) OF 24 COMPOSED OF RX(9), RX(2)

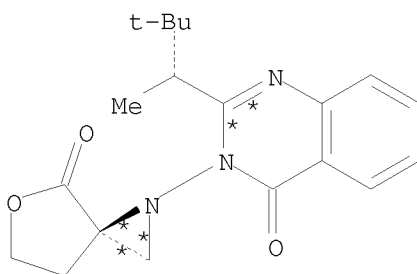
RX(16) 2 P + 2 B ==> C + G



10/ 562,112



C

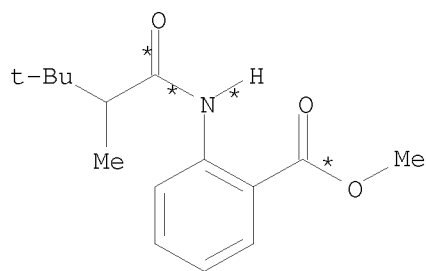


G

RX(9) RCT P 115855-35-1  
PRO A 116065-10-2  
SOL 64-17-5 EtOH

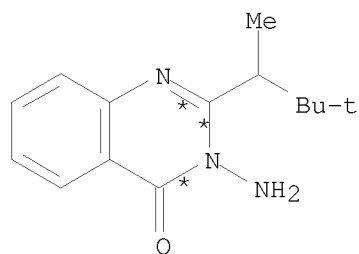
RX(2) RCT A 116065-10-2, B 547-65-9  
RGT D 546-67-8 Pb(OAc)4  
PRO C 105983-10-6, G 105983-09-3  
SOL 75-09-2 CH2Cl2

RX(17) OF 24 COMPOSED OF RX(5), RX(9)  
RX(17) 2 O ==> A



2 O

2  
STEPS  
→



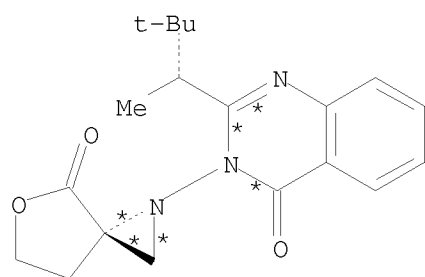
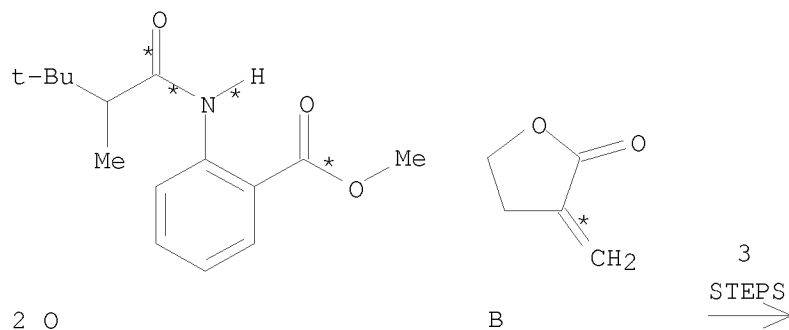
A

RX(5) RCT O 115875-69-9  
RGT Q 302-01-2 N2H4  
PRO A 116065-10-2, P 115855-35-1  
SOL 64-17-5 EtOH

RX(9) RCT P 115855-35-1  
PRO A 116065-10-2  
SOL 64-17-5 EtOH

RX(21) OF 24 COMPOSED OF RX(5), RX(9), RX(1)  
RX(21) 2 O + B ==> C

10/ 562,112

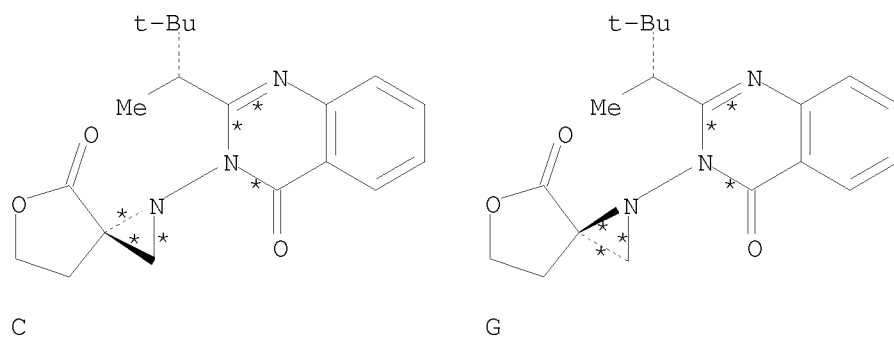
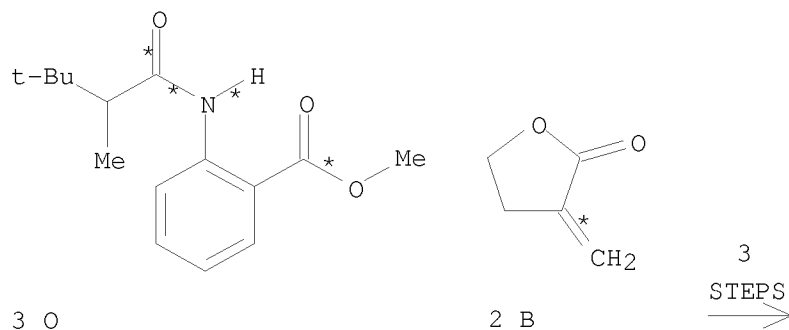


C  
YIELD 72%

RX(5)	RCT	O 115875-69-9
	RGT	Q 302-01-2 N <sub>2</sub> H <sub>4</sub>
	PRO	A 116065-10-2, P 115855-35-1
	SOL	64-17-5 EtOH
RX(9)	RCT	P 115855-35-1
	PRO	A 116065-10-2
	SOL	64-17-5 EtOH
RX(1)	RCT	A 116065-10-2, B 547-65-9
	RGT	D 546-67-8 Pb(OAc) <sub>4</sub> , E 76-05-1 F <sub>3</sub> CCO <sub>2</sub> H
	PRO	C 105983-10-6
	SOL	75-09-2 CH <sub>2</sub> Cl <sub>2</sub>

RX(22) OF 24 COMPOSED OF RX(5), RX(9), RX(2)  
 RX(22) 3 O + 2 B ==> C + G





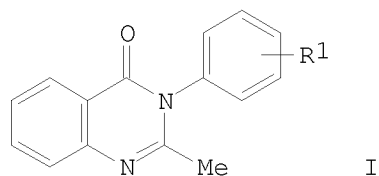
RX(5)      RCT   O 115875-69-9  
              RGT   Q 302-01-2 N2H4  
              PRO   A 116065-10-2, P 115855-35-1  
              SOL   64-17-5 EtOH

RX(9)	RCT	P 115855-35-1
	PRO	A 116065-10-2
	SOL	64-17-5 EtOH

RX(2) RCT A 116065-10-2, B 547-65-9  
RGT D 546-67-8 Pb(OAc)4  
PRO C 105983-10-6, G 105983-09-3  
SOL 75-09-2 CH2Cl2

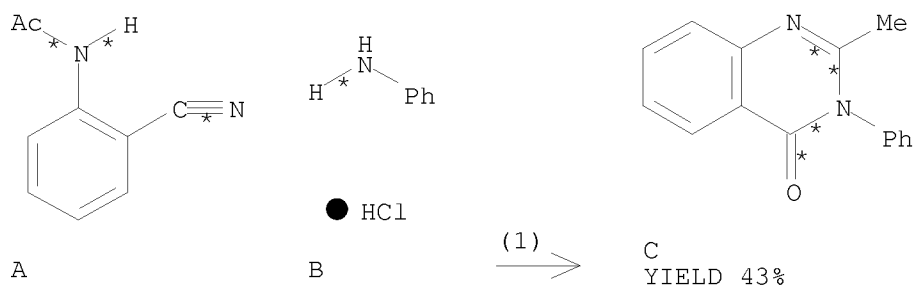
```
L3      ANSWER 178 OF 258      CASREACT  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:      108:186690  CASREACT
TITLE:      Phosphorus pentoxide in organic synthesis.  XXX.  New
              synthesis of 4(3H)-quinazolinones
AUTHOR(S):      Hilmy, Khalid Mohamed Hassan; Mogensen, Joergen;
              Pedersen, Erik B.
CORPORATE SOURCE:      Dep. Chem., Odense Univ., Odense, DK-5230, Den.
SOURCE:      Acta Chemica Scandinavica, Series B: Organic
              Chemistry and Biochemistry (1987), B41(6), 467-8
              CODEN: ACBOCV; ISSN: 0302-4369
```

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



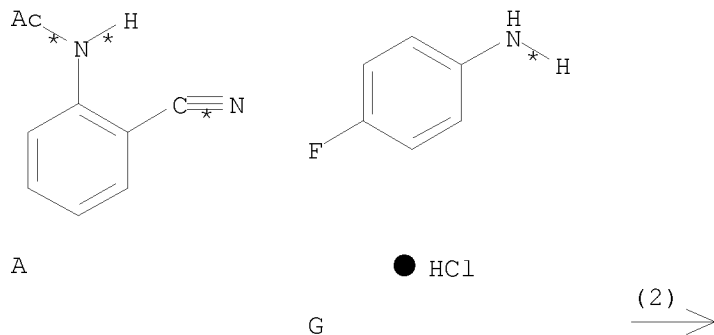
AB Aniline salts  $R_1C_6H_4NH_2 \cdot HCl$  ( $R_1 = H, F, Cl, Me$ ) were heated with  $P_2O_5$ , water, and  $N,N$ -dimethylcyclohexylamine hydrochloride to give quinazolinones I.

RX(1) OF 10      A + B ==> C

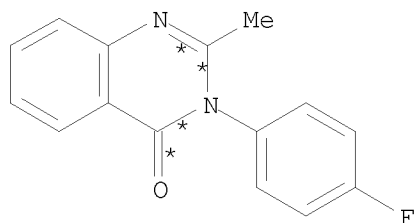


RX(1)      RCT    A 25116-00-1, B 142-04-1  
 RGT    D 1314-56-3  $P_2O_5$ , E 2498-24-0  $Me_2NC_6H_{11} \cdot HCl$ , F 7732-18-5 Water  
 PRO    C 2385-23-1

RX(2) OF 10      A + G ==> H



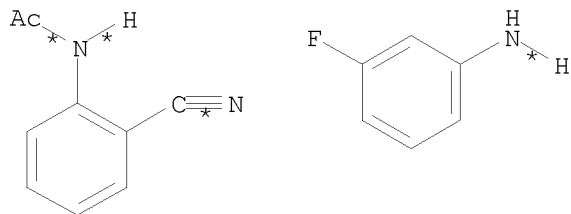
10/ 562,112



H  
YIELD 37%

RX(2) RCT A 25116-00-1, G 2146-07-8  
RGT D 1314-56-3 P2O5, E 2498-24-0 Me2NC6H11.HCl, F 7732-18-5 Water  
PRO H 1897-80-9

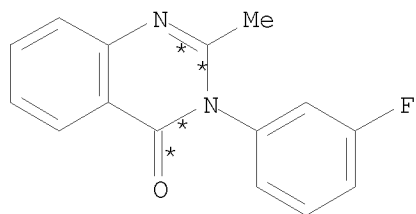
RX(3) OF 10 A + I ==> J



A ● HCl

I

(3) ➞

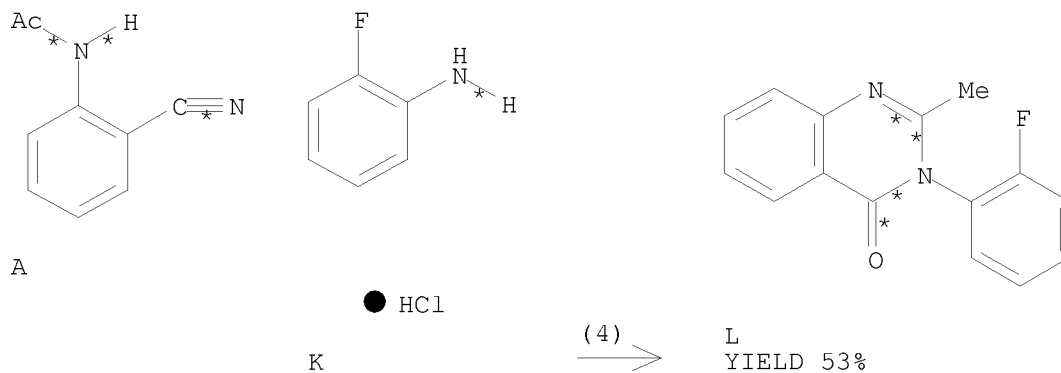


J  
YIELD 46%

RX(3) RCT A 25116-00-1, I 1993-09-5  
RGT D 1314-56-3 P2O5, E 2498-24-0 Me2NC6H11.HCl, F 7732-18-5 Water  
PRO J 1789-04-4

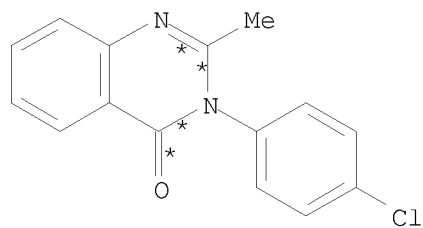
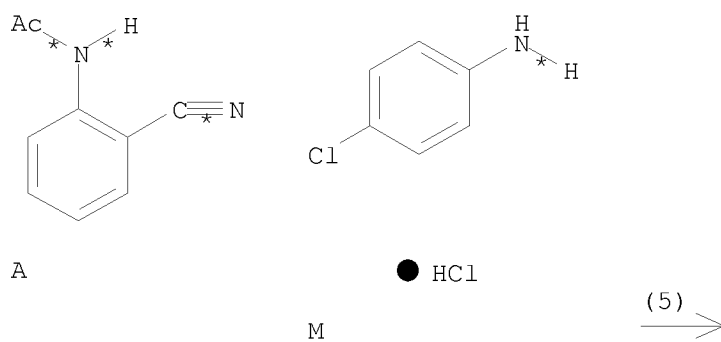
RX(4) OF 10 A + K ==> L

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RX(4) RCT A 25116-00-1, K 51085-49-5  
RGT D 1314-56-3 P2O5, E 2498-24-0 Me2NC6H11.HCl, F 7732-18-5 Water  
PRO L 1897-87-6

RX(5) OF 10 A + M ==> N



N  
YIELD 50%

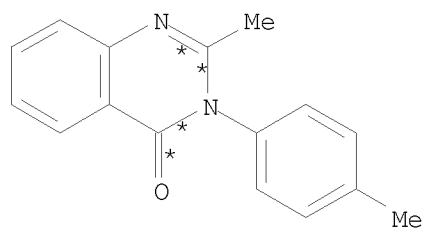
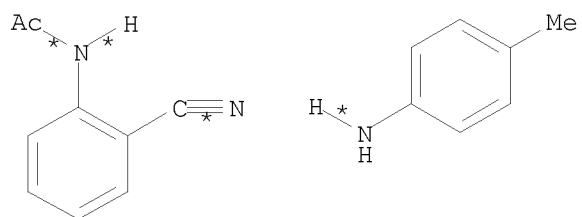
RX(5) RCT A 25116-00-1, M 20265-96-7  
RGT D 1314-56-3 P2O5, E 2498-24-0 Me2NC6H11.HCl, F 7732-18-5 Water  
PRO N 1788-93-8

RX(6) OF 10 A + O ==> P



10/ 562,112

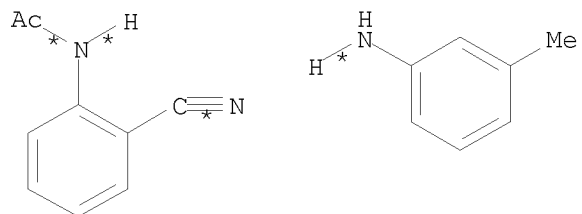
RX(8) OF 10      A + S ==> T



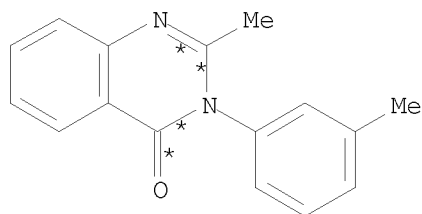
T  
YIELD 33%

RX(8)      RCT    A 25116-00-1, S 540-23-8  
RGT    D 1314-56-3 P2O5, E 2498-24-0 Me2NC6H11.HCl, F 7732-18-5 Water  
PRO    T 22316-59-2

RX(9) OF 10      A + U ==> V



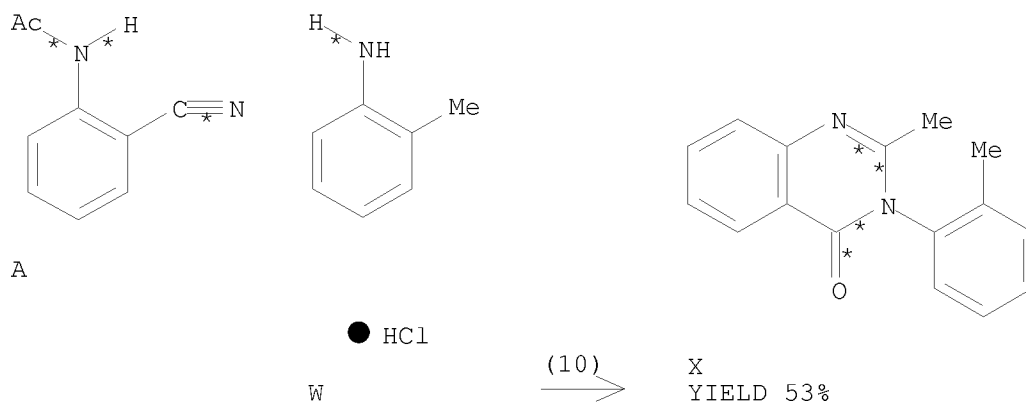
10/ 562,112



V  
YIELD 40%

RX(9) RCT A 25116-00-1, U 638-03-9  
RGT D 1314-56-3 P2O5, E 2498-24-0 Me2NC6H11.HCl, F 7732-18-5 Water  
PRO V 22288-99-9

RX(10) OF 10 A + W ==> X



RX(10) RCT A 25116-00-1, W 636-21-5  
RGT D 1314-56-3 P2O5, E 2498-24-0 Me2NC6H11.HCl, F 7732-18-5 Water  
PRO X 72-44-6

L3 ANSWER 179 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 108:56047 CASREACT  
TITLE: Some reactions of  
N-[(3,4-dimethylbenzoyl)acryloyl]anthranilic acid and  
its derivatives  
AUTHOR(S): Soliman, E. A.; Hataba, A. M.; Attia, I. A.;  
El-Shahed, F. A.; Mousa, H. A.  
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt  
SOURCE: Journal of the Chemical Society of Pakistan (1987),  
9(1), 19-34  
CODEN: JCSPDF; ISSN: 0253-5106  
DOCUMENT TYPE: Journal

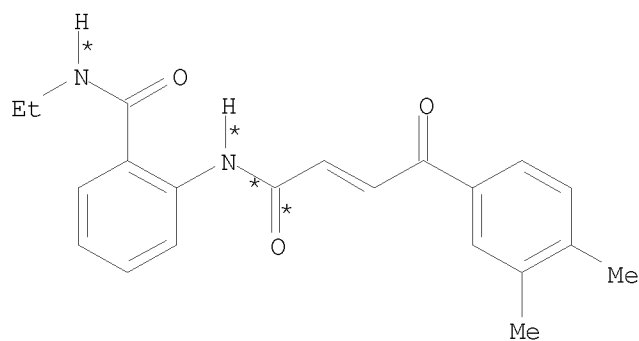
10/ 562,112

LANGUAGE: English  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

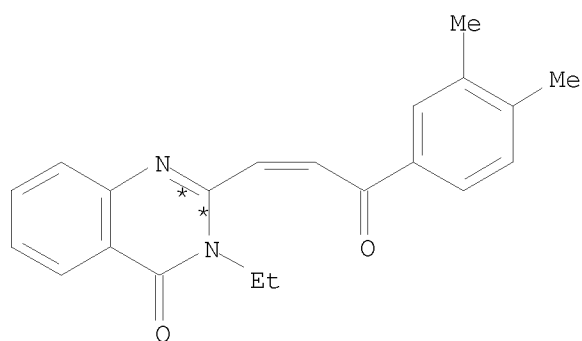
AB Cyclization of anthranilic acid derivative I with  $\text{RNHC}(:\text{Z})\text{NH}_2$  ( $\text{R} = \text{H}$ ,  $\text{Z} = \text{O}$ ,  $\text{S}$ ;  $\text{R} = \text{PhCH}_2$ ,  $\text{Z} = \text{S}$ ) and with  $\text{Ac}_2\text{O}$  gave pyrimidines II ( $\text{R} = \text{H}$ ,  $\text{PhCH}_2$ ;  $\text{Z} = \text{O}$ ,  $\text{S}$ ) and benzoxazinone III, resp. Cyclocondensation of III with  $\text{N}_2\text{H}_4$  gave aminoquinazolinone IV ( $\text{R}_1 = \text{H}$ ). Condensation of III with  $\text{N}_2\text{H}_4$  in the presence of  $\text{R}_2\text{CO}_2\text{H}$  ( $\text{R}_2 = \text{H}$ ,  $\text{Me}$ ,  $\text{Et}$ ,  $\text{Pr}$ ) gave IV ( $\text{R}_1 = \text{COR}_2$ ). Some reactions of IV ( $\text{R}_1 = \text{H}$ ) were also investigated.

RX(12) OF 122 ...V ==> AC



V

(12)  $\longrightarrow$



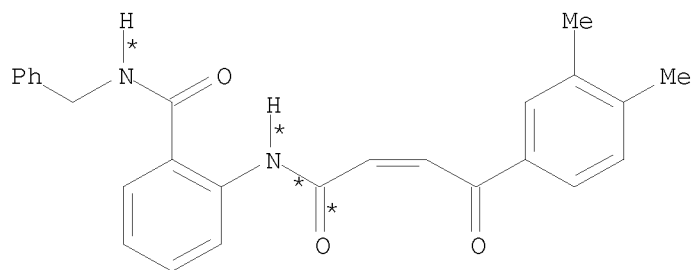
AC  
YIELD 50%

RX(12) RCT V 112371-81-0  
RGT R 108-24-7  $\text{Ac}_2\text{O}$   
PRO AC 112371-77-4  
SOL 108-24-7  $\text{Ac}_2\text{O}$



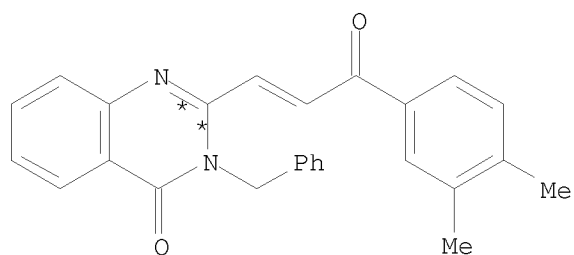
10/ 562,112

RX(14) OF 122 ...Z ==> AD



Z

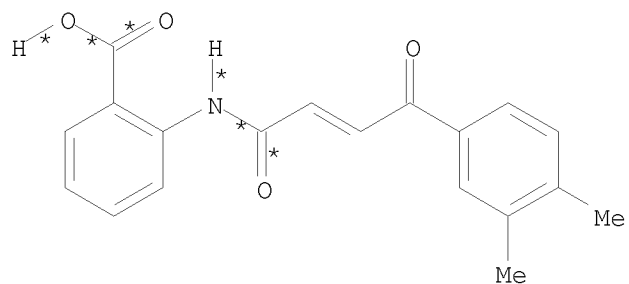
(14)



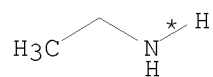
AD  
YIELD 55%

RX(14)      RCT    Z 112371-79-6  
              RGT    R 108-24-7 Ac2O  
              PRO    AD 112371-76-3  
              SOL    108-24-7 Ac2O

RX(49) OF 122 COMPOSED OF RX(6), RX(13)  
RX(49)      C + U ==> AC



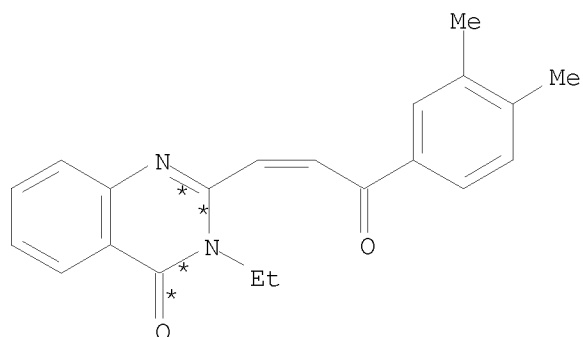
C



U

2  
STEPS

10/ 562,112

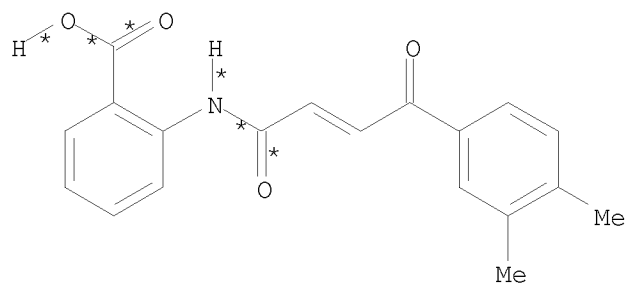


AC  
YIELD 50%

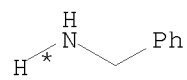
RX(6)      RCT    C 112371-88-7  
              RGT    R 108-24-7 Ac2O  
              PRO    Q 112371-83-2  
              SOL    108-24-7 Ac2O

RX(13)      RCT    Q 112371-83-2, U 75-04-7  
              RGT    AA 124-40-3 Me2NH  
              PRO    AC 112371-77-4

RX(50) OF 122 COMPOSED OF RX(6), RX(15)  
RX(50)      C    +    Y    ==>    AD



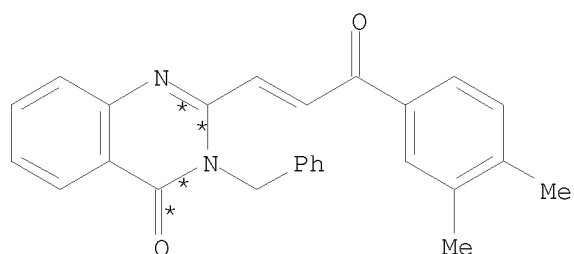
C



Y

2  
STEPS  
→

10/ 562,112

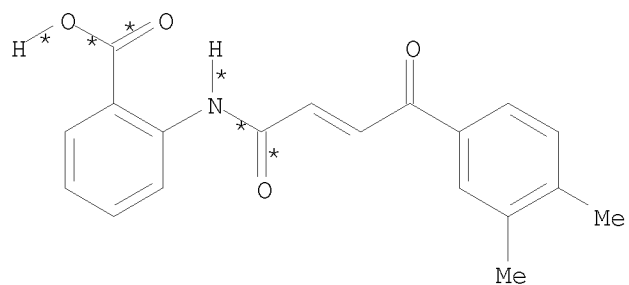


AD  
YIELD 55%

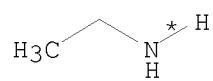
RX(6)      RCT    C 112371-88-7  
              RGT    R 108-24-7 Ac2O  
              PRO    Q 112371-83-2  
              SOL    108-24-7 Ac2O

RX(15)      RCT    Q 112371-83-2, Y 100-46-9  
              RGT    AA 124-40-3 Me2NH  
              PRO    AD 112371-76-3

RX(93) OF 122 COMPOSED OF RX(6), RX(8), RX(12)  
RX(93)      C    +    U    ==>    AC



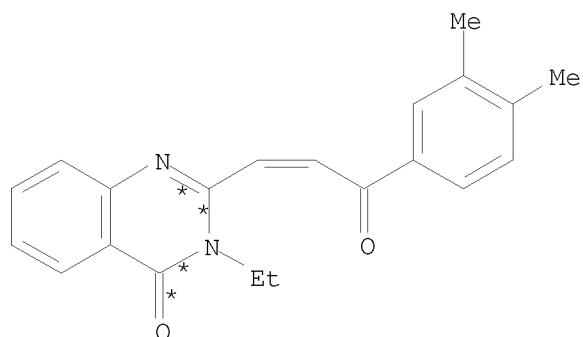
C



U

3  
STEPS  
→

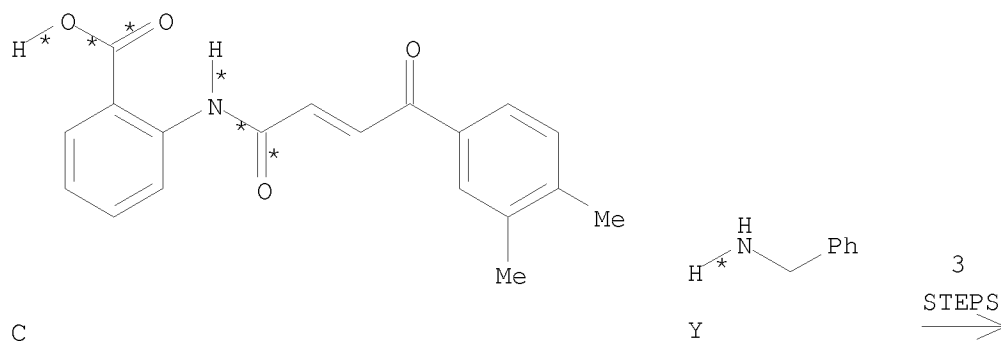
10/ 562,112

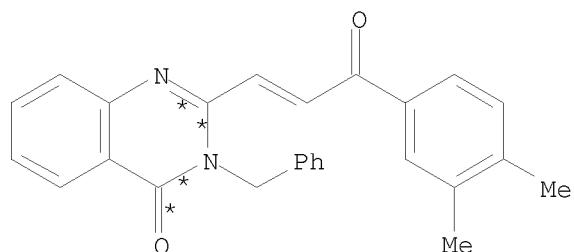


AC  
YIELD 50%

RX(6)	RCT	C	112371-88-7
	RGT	R	108-24-7 Ac2O
	PRO	Q	112371-83-2
	SOL		108-24-7 Ac2O
RX(8)	RCT	Q	112371-83-2, U 75-04-7
	PRO	V	112371-81-0
	SOL		64-17-5 EtOH
RX(12)	RCT	V	112371-81-0
	RGT	R	108-24-7 Ac2O
	PRO	AC	112371-77-4
	SOL		108-24-7 Ac2O

RX(94) OF 122 COMPOSED OF RX(6), RX(10), RX(14)  
RX(94) C + Y ==> AD

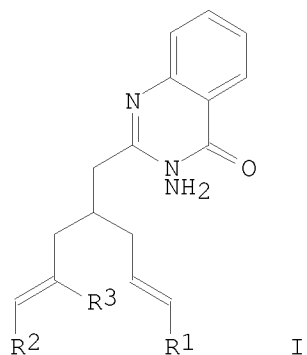




AD  
YIELD 55%

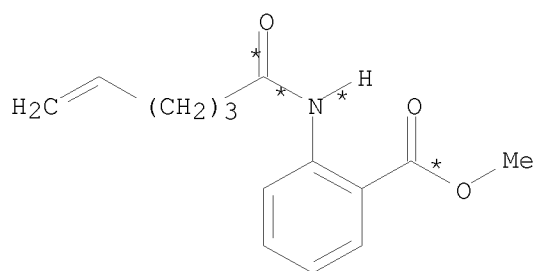
RX(6)	RCT	C 112371-88-7
	RGT	R 108-24-7 Ac2O
	PRO	Q 112371-83-2
	SOL	108-24-7 Ac2O
RX(10)	RCT	Q 112371-83-2, Y 100-46-9
	PRO	Z 112371-79-6
	SOL	64-17-5 EtOH
RX(14)	RCT	Z 112371-79-6
	RGT	R 108-24-7 Ac2O
	PRO	AD 112371-76-3
	SOL	108-24-7 Ac2O

L3 ANSWER 180 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 108:56028 CASREACT  
 TITLE: Intramolecular reactions of N-nitrenes. Description of the transition state geometry for addition to alkenes  
 AUTHOR(S): Atkinson, Roberts S.; Grimshire, Michael J.  
 CORPORATE SOURCE: Dep. Chem., Univ. Leicester, Leicester, LE1 7RH, UK  
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (5), 1127-37  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



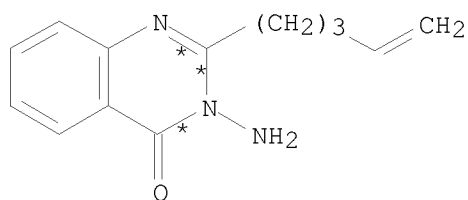
AB Oxidation of the N-aminoquinazolones I ( $R_1 = R_3 = H$ ,  $R_2 = Ph$ ;  $R_1 = R_3 = Me$ ,  $R_2 = H$ ) by  $Pb(OAc)_4$  generates the corresponding N-nitrenes which add intramolecularly to both double bonds. Although nitrene addition is stereospecifically cis, both faces of each double bond are attacked and consequently stereoisomers are formed. From the different selectivity of the N-nitrenes for the two double bonds in I and from a consideration of the stereoisomer ratios, a transition-state is proposed for the concerted addition of the N-nitrene to the double bonds in (I).

RX(26) OF 204 ...AT ==> AV...



AT

(26)  $\longrightarrow$



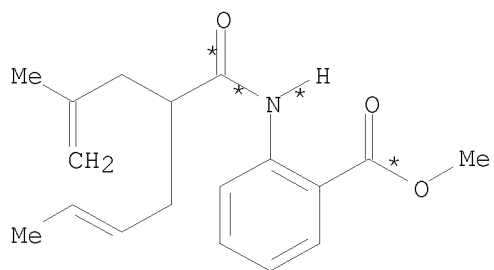
AV  
YIELD 80%

RX(26) RCT AT 112391-61-4

10/ 562,112

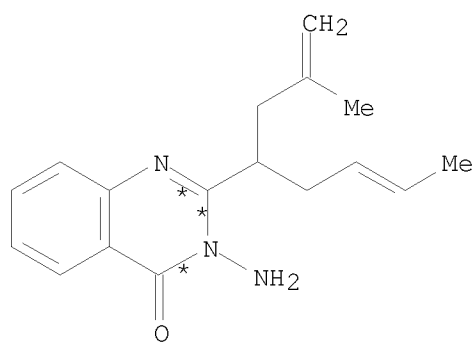
RGT AW 302-01-2 N2H4  
PRO AV 112391-72-7  
SOL 64-17-5 EtOH

RX(27) OF 204 ...AX ==> AY...



AX

(27)

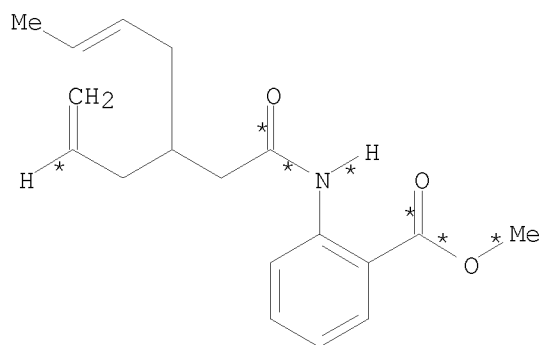


AY  
YIELD 90%

RX(27) RCT AX 112391-62-5  
RGT AW 302-01-2 N2H4  
PRO AY 112391-73-8  
SOL 64-17-5 EtOH

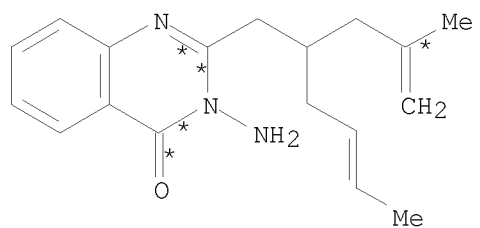
RX(28) OF 204 ...AZ ==> BA...

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AZ

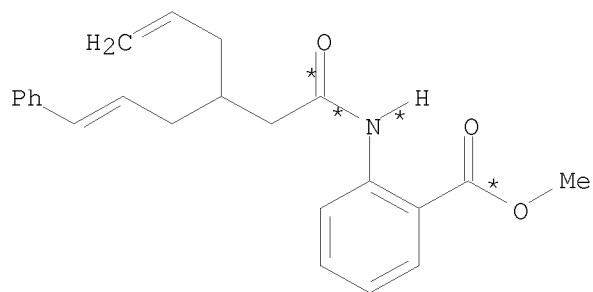
(28)  $\longrightarrow$



BA

RX(28)     RCT    AZ 112391-63-6  
               RGT    AW 302-01-2 N2H4  
               PRO    BA 101126-05-0  
               SOL    64-17-5 EtOH

RX(29) OF 204     ...BB ==> BC...

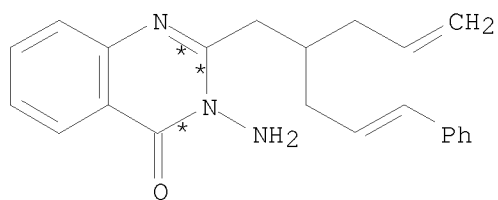


BB

(29)  $\longrightarrow$



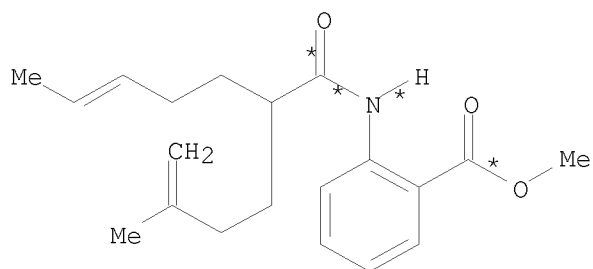
10/ 562,112



BC  
YIELD 41%

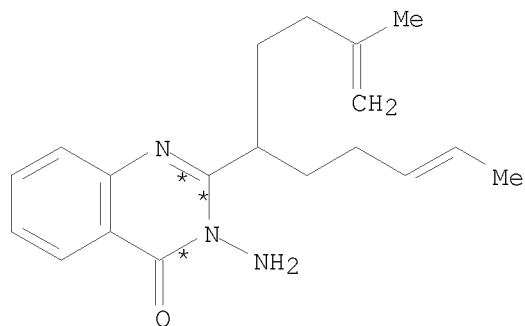
RX(29)      RCT    BB 112391-64-7  
              RGT    AW 302-01-2 N2H4  
              PRO    BC 101126-02-7  
              SOL    64-17-5 EtOH

RX(30) OF 204      ...BD ==> BE...



BD

(30) →

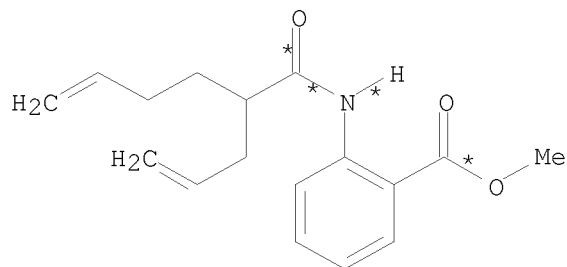


BE  
YIELD 47%

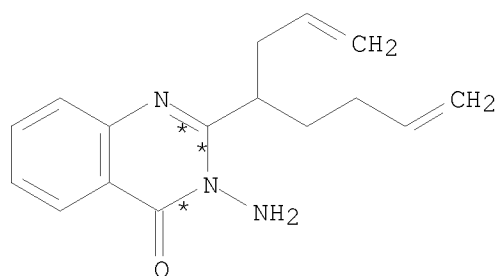
RX(30)      RCT    BD 112391-65-8  
              RGT    AW 302-01-2 N2H4  
              PRO    BE 112391-74-9  
              SOL    64-17-5 EtOH

10/ 562,112

RX(31) OF 204 ...BF ==> BG...



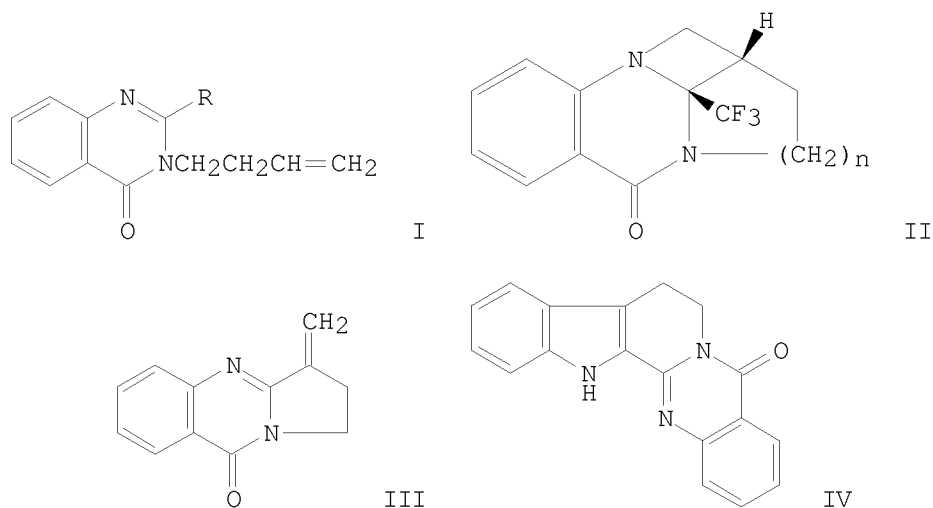
BF



BG  
YIELD 56%

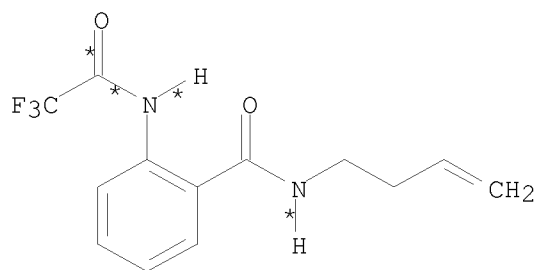
RX(31)      RCT    BF 112391-66-9  
             RGT    AW 302-01-2 N2H4  
             PRO    BG 112391-75-0  
             SOL    64-17-5 EtOH

L3    ANSWER 181 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER:      107:134232    CASREACT  
TITLE:                    Cycloadditions in syntheses. Part XXX. Photoaddition  
                             of 4(3H)-quinazolinone derivatives to olefins:  
                             effects of the 2-substituent  
AUTHOR(S):                Kaneko, Chikara; Kasai, Kouichi; Katagiri, Nobuya;  
                             Chiba, Takuo  
CORPORATE SOURCE:        Pharm. Inst., Tohoku Univ., Sendai, 980, Japan  
SOURCE:                    Chemical & Pharmaceutical Bulletin (1986), 34(9),  
                             3672-81  
                             CODEN: CPBTAL; ISSN: 0009-2363  
DOCUMENT TYPE:            Journal  
LANGUAGE:                  English  
GI



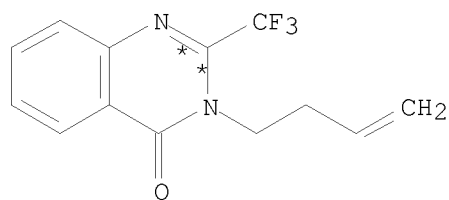
AB The photochem. behavior of 3-(3-butenyl)-4(3H)-quinazolinones I ( $R = H, Cl, F_3C$ ) was examined in MeOH at a variety of wavelengths (254, 300, and 350 nm). The intramol. 2 + 2 photoadducts II ( $n = 1, 2$ ) were obtained only when I ( $R = F_3C$ ) and its higher methylene homolog were irradiated. Though the 2-unsubstituted quinazolinone I ( $R = H$ ) was photostable I ( $R = Cl$ ) afforded the cyclized product (III) via homolytic fission of the C-Cl bond. An enhancement of the photocycloaddn. reactivity of the C:N bond in the quinazolinone ring by introduction of a trifluoromethyl group was also demonstrated by the formation of the intermol. adducts from 2-trifluoromethyl-4(3H)-quinazolinone by irradiation in the presence of olefins. The reactions due to C-N bond fission of the azetidine ring in these adducts are also described. Rutecarpine (IV) was synthesized by irradiation of 2-chloro-3-[2-(indol-3-yl)ethyl]-4-(3H)-quinazolinone.

RX(8) OF 63      ...T ==> V...



(8)  $\longrightarrow$

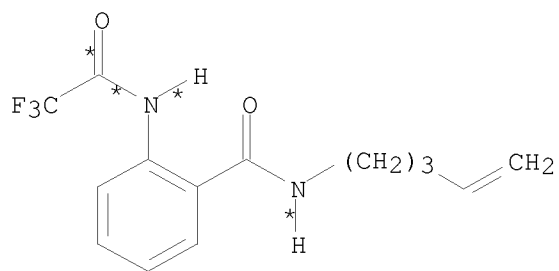
10/ 562,112



V  
YIELD 85%

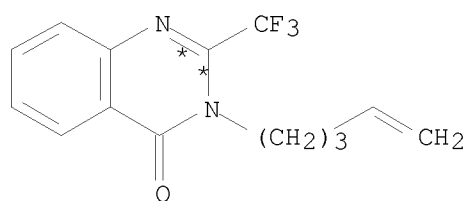
RX(8) RCT T 109071-12-7  
PRO V 109071-13-8

RX(14) OF 63 ...AG ==> AH...



AG

(14)

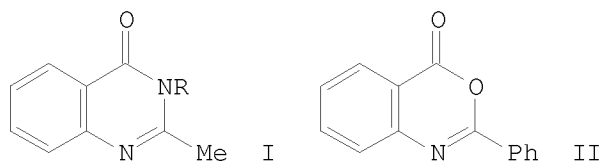


AH  
YIELD 74%

RX(14) RCT AG 109071-16-1  
PRO AH 109071-17-2

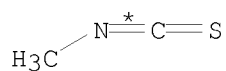
L3 ANSWER 182 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 107:77742 CASREACT  
TITLE: One-pot synthesis of 2,3-disubstituted

AUTHOR(S): Ashare, Ram; Mukerjee, Arya K.  
 CORPORATE SOURCE: Fac. Sci., Banaras Hindu Univ., Yaranasi, 221 005, India  
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1986), 25B(11), 1180-1  
 CODEN: IJSBDB; ISSN: 0376-4699  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

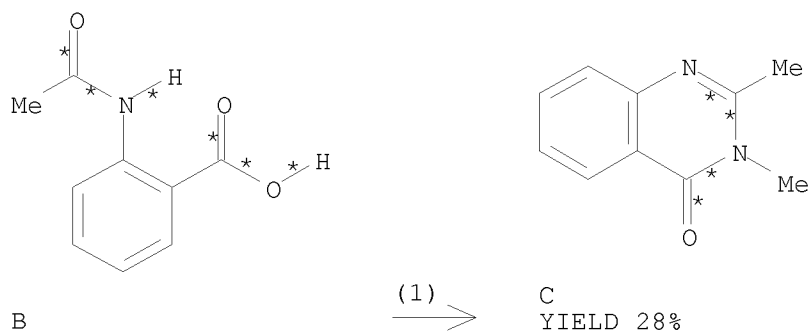


AB The condensation of N-acetylanthranilic acid with Me and Ph isothiocyanates affords the corresponding 3-substituted 2-methylquinazolin-4-ones I (R = Me, Ph), N-benzoylanthranilic acid reacts with these isothiocyanates to give 2-phenyl-3,1-benzoxazin-4-one II and 2-BzNHC6H4CONHPh resp.

RX(1) OF 4            A + B ==> C

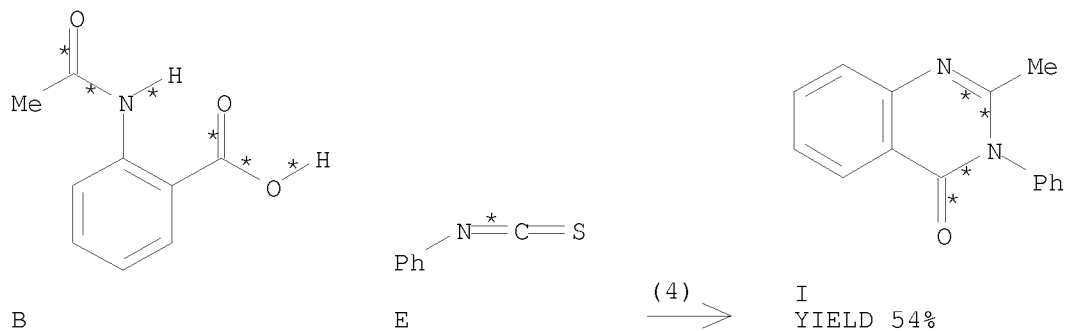


A



RX(1)            RCT    A 556-61-6, B 89-52-1  
                   RGT    D 110-86-1 Pyridine  
                   PRO    C 1769-25-1

RX(4) OF 4            B + E ==> I

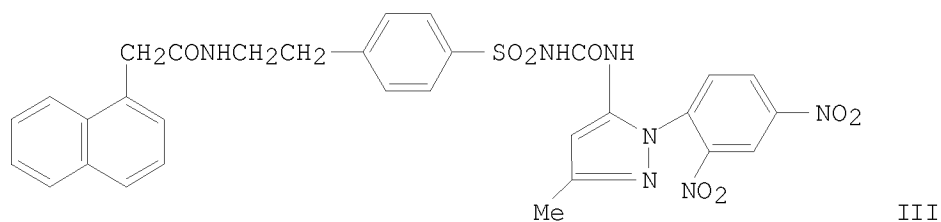
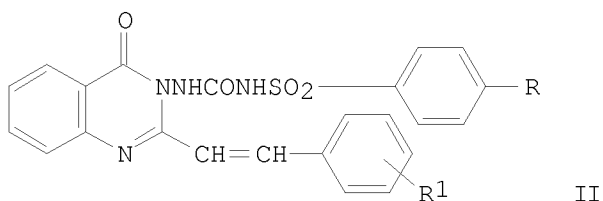
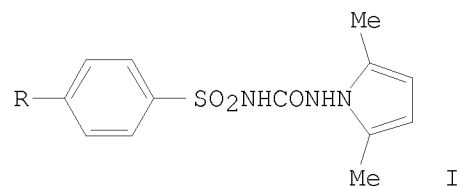


RX(4)       RCT   B 89-52-1, E 103-72-0  
             RGT   D 110-86-1 Pyridine  
             PRO   I 2385-23-1

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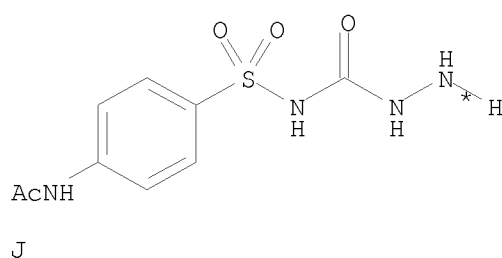
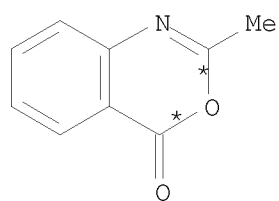
L3      ANSWER 183 OF 258      CASREACT  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:              107:58968  CASREACT
TITLE:                          Synthesis of some new substituted sulfonylureas as
                                oral hypoglycemic agents
AUTHOR(S):                     Husain, M. I.; Srivastava, V. P.
CORPORATE SOURCE:              Dep. Chem., Lucknow Univ., Lucknow, 226 007, India
SOURCE:                         Indian Journal of Chemistry, Section B: Organic
                                Chemistry Including Medicinal Chemistry (1986),
                                25B(9), 934-8
                                CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE:                  Journal
LANGUAGE:                       English
GI

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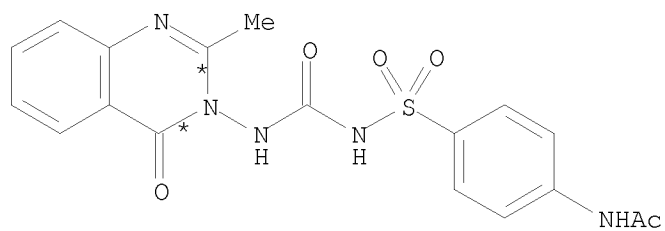
AB The title compds., e.g. I (R = H, Me, MeO, AcNH), II (R1 = 4-Me, 4-MeO, 4-Cl, 4-NO<sub>2</sub>) and III were prepared and their hypoglycemic activity evaluated. Some of these compds., when screened on albino rats at an oral dose of 250 mg/kg body weight, reduce the blood sugar to a significant extent.

RX(12) OF 107 ...N + J ==> V...



(12)  $\longrightarrow$

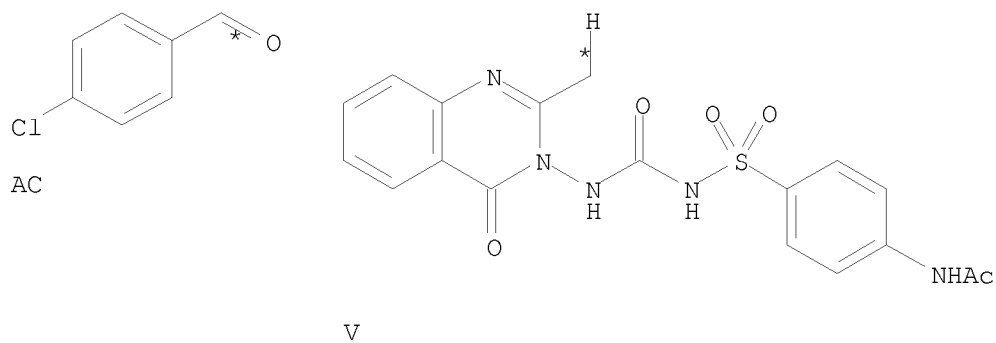
10/ 562,112



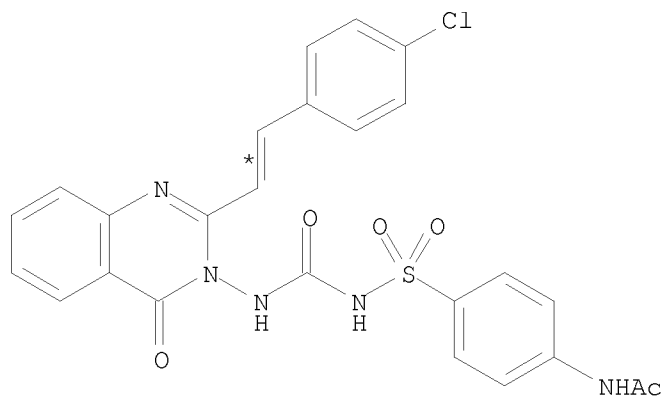
V  
YIELD 62%

RX(12) RCT N 525-76-8, J 76983-56-7  
PRO V 109274-28-4  
SOL 110-86-1 Pyridine

RX(19) OF 107 ...AC + V ==> AG



(19)  
→



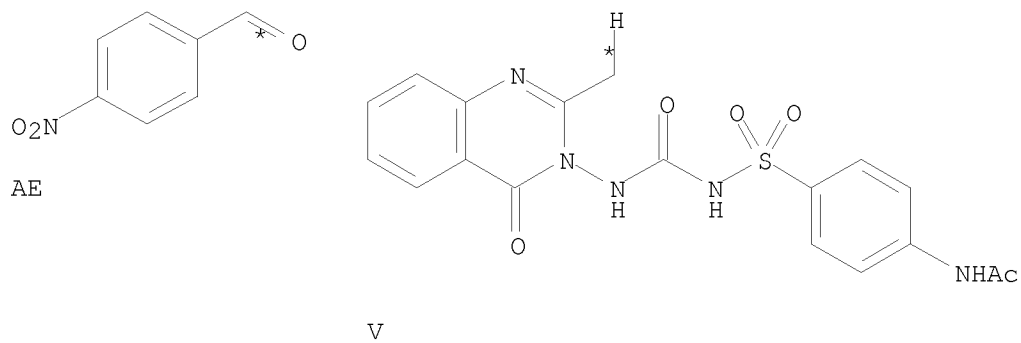
AG  
YIELD 84%



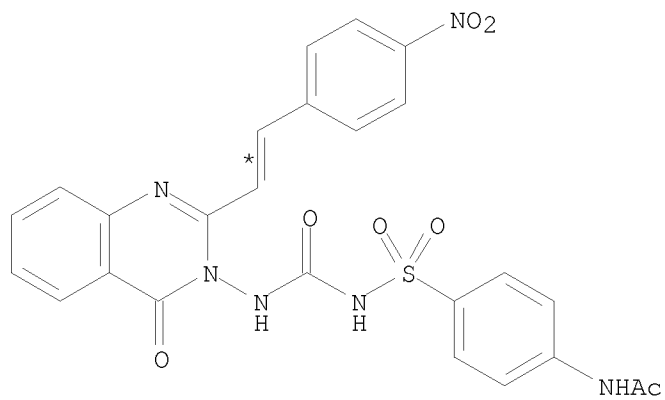
10/ 562,112

RX(19)      RCT    AC 104-88-1, V 109274-28-4  
              RGT    M 64-19-7 AcOH  
              PRO    AG 109274-46-6  
              SOL    64-17-5 EtOH

RX(20) OF 107      ...AE + V ==> AH



(20)  $\longrightarrow$

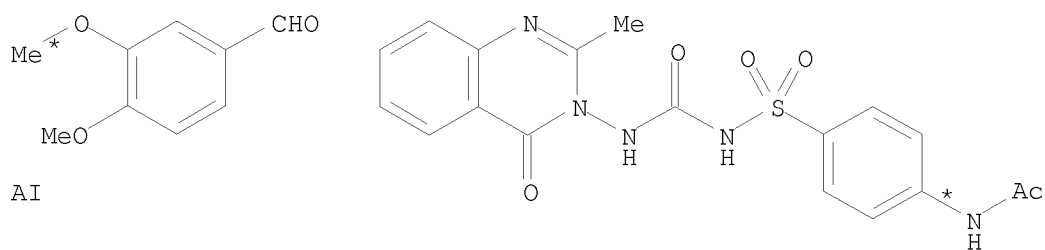


AH  
YIELD 76%

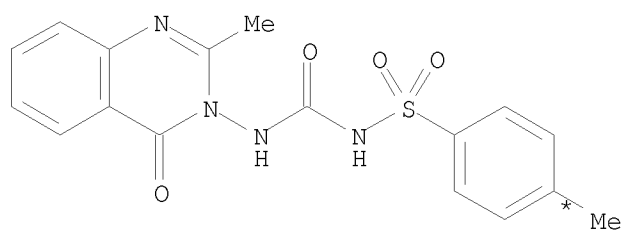
RX(20)      RCT    AE 555-16-8, V 109274-28-4  
              RGT    M 64-19-7 AcOH  
              PRO    AH 109274-47-7  
              SOL    64-17-5 EtOH

RX(21) OF 107      ...AI + V ==> R...

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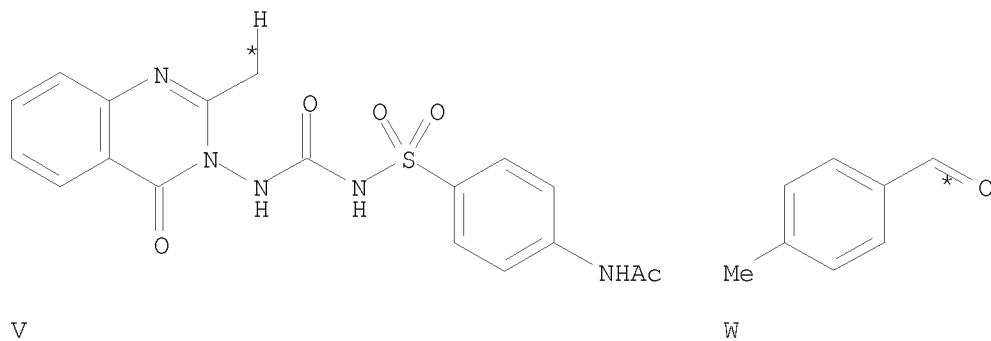


(21)  $\longrightarrow$



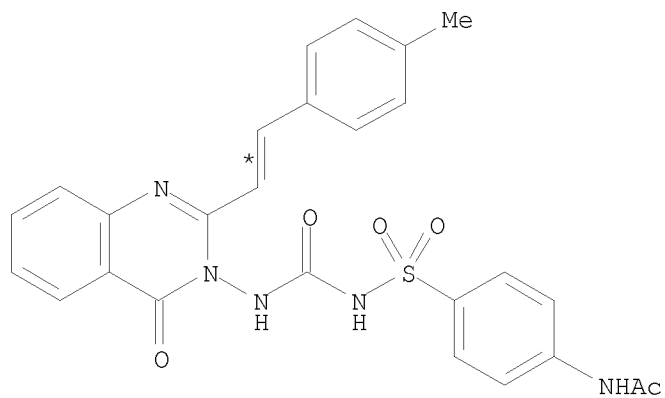
RX(21)     RCT    AI 120-14-9, V 109274-28-4  
              RGT    M 64-19-7 AcOH  
              PRO    R 109274-27-3  
              SOL    64-17-5 EtOH

RX(23) OF 107     ...V + W ==> AK



(23)  $\longrightarrow$

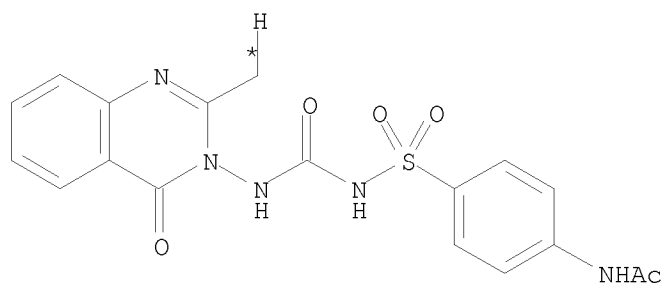
10/ 562,112



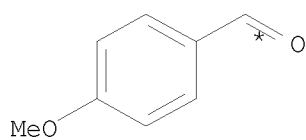
AK  
YIELD 86%

RX(23)      RCT    V 109274-28-4, W 104-87-0  
              RGT    M 64-19-7 AcOH  
              PRO    AK 109274-44-4  
              SOL    64-17-5 EtOH

RX(25) OF 107      ...V + Y ==> AM



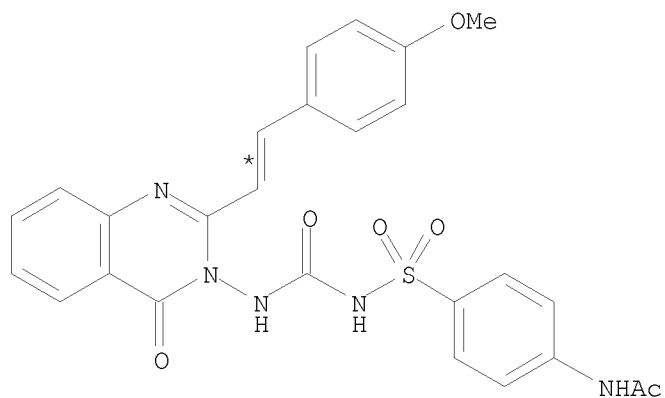
V



Y

(25)  
→

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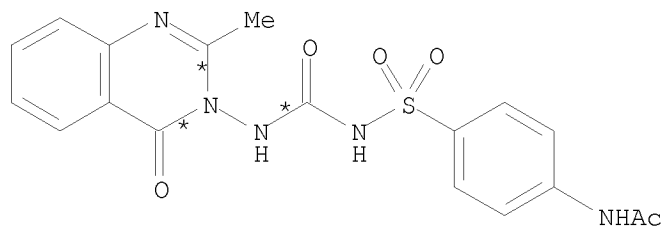
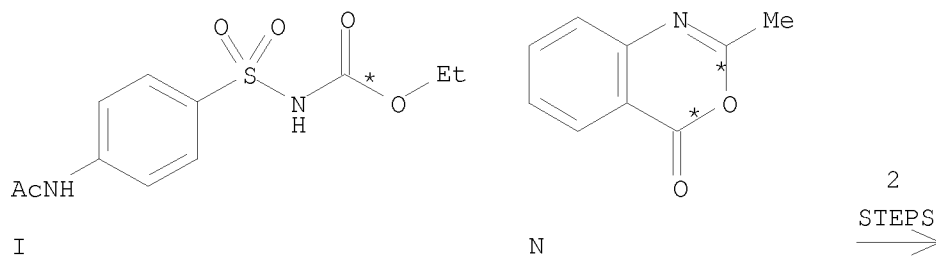
AM

YIELD 76%

RX(25) RCT V 109274-28-4, Y 123-11-5  
RGT M 64-19-7 AcOH  
PRO AM 109274-45-5  
SOL 64-17-5 EtOH

RX(45) OF 107 COMPOSED OF RX(4), RX(12)

RX(45) I + N ==> V



V

YIELD 62%

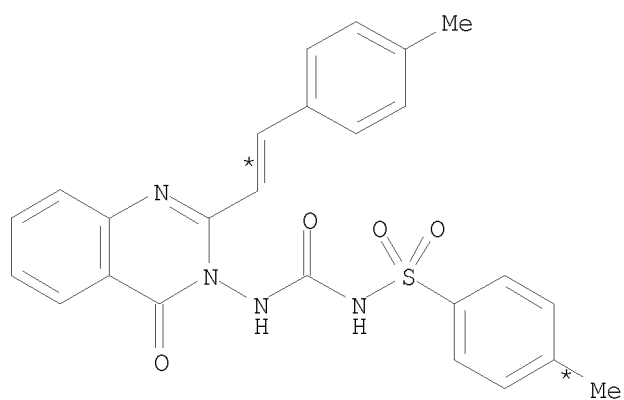
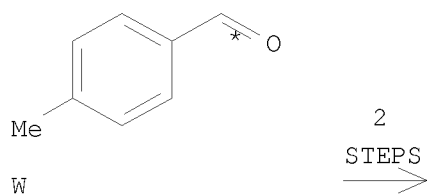
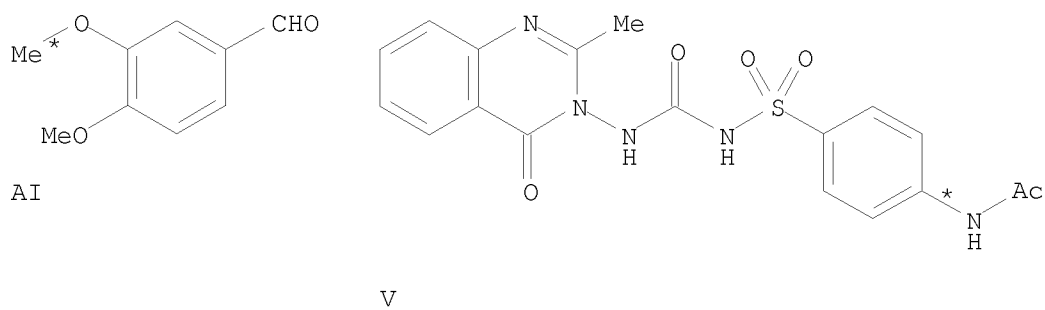
RX(4) RCT I 13945-59-0  
RGT C 302-01-2 N2H4

10/ 562,112

PRO J 76983-56-7  
SOL 64-17-5 EtOH

RX(12) RCT N 525-76-8, J 76983-56-7  
PRO V 109274-28-4  
SOL 110-86-1 Pyridine

RX(56) OF 107 COMPOSED OF RX(21), RX(15)  
RX(56) AI + V + W ==> AA



AA  
YIELD 54%

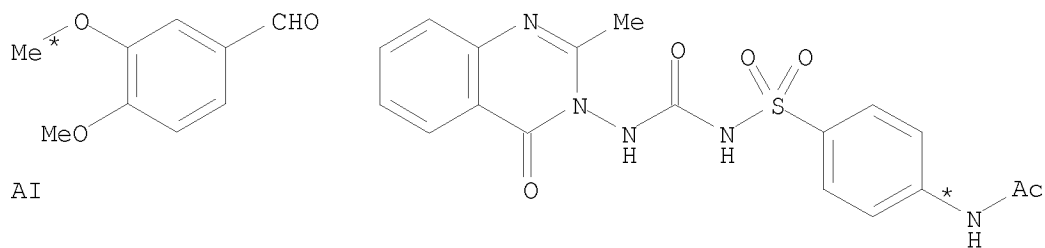
RX(21) RCT AI 120-14-9, V 109274-28-4  
RGT M 64-19-7 AcOH  
PRO R 109274-27-3

10/ 562,112

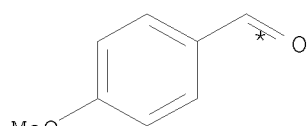
SOL 64-17-5 EtOH

RX(15) RCT W 104-87-0, R 109274-27-3  
RGT M 64-19-7 AcOH  
PRO AA 109274-34-2  
SOL 64-17-5 EtOH

RX(57) OF 107 COMPOSED OF RX(21), RX(16)  
RX(57) AI + V + Y ==> AB

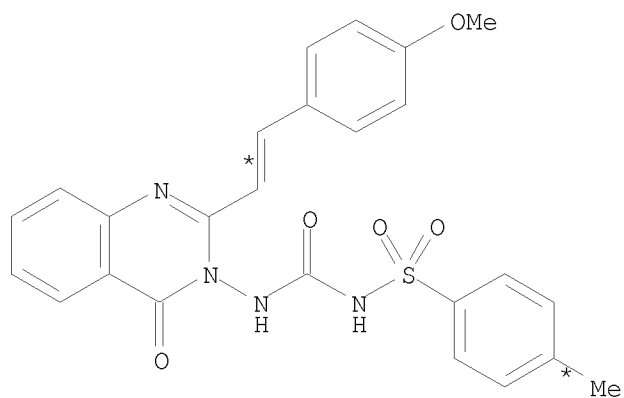


V



Y

2  
STEPS  
→



AB  
YIELD 60%

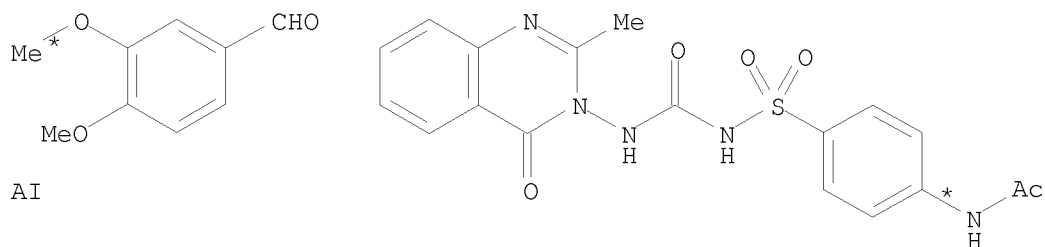
RX(21) RCT AI 120-14-9, V 109274-28-4  
RGT M 64-19-7 AcOH  
PRO R 109274-27-3  
SOL 64-17-5 EtOH

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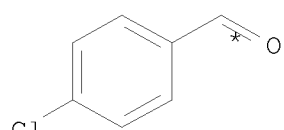
RX(16) RCT Y 123-11-5, R 109274-27-3  
RGT M 64-19-7 AcOH  
PRO AB 109274-35-3  
SOL 64-17-5 EtOH

RX(58) OF 107 COMPOSED OF RX(21), RX(26)

RX(58) AI + V + AC ==> AN

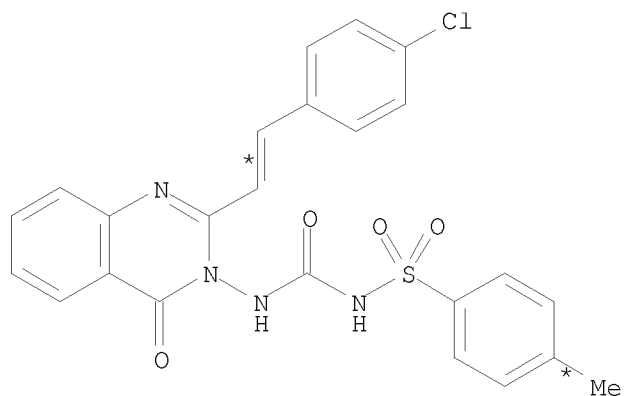


V



AC

2  
STEPS  
→



AN

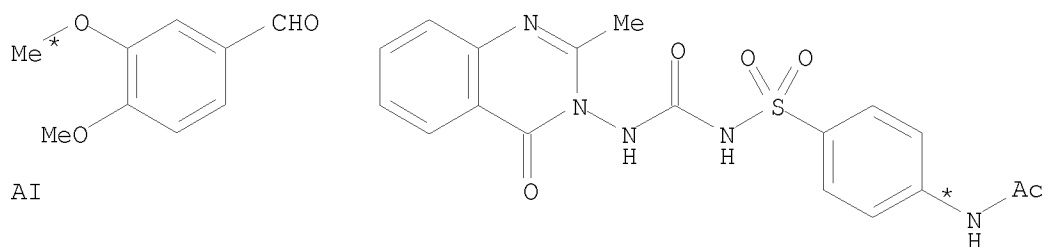
YIELD 68%

RX(21) RCT AI 120-14-9, V 109274-28-4  
RGT M 64-19-7 AcOH  
PRO R 109274-27-3  
SOL 64-17-5 EtOH

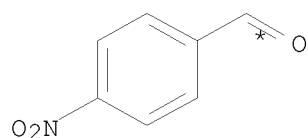
10/ 562,112

RX(26)      RCT    R 109274-27-3, AC 104-88-1  
              RGT    M 64-19-7 AcOH  
              PRO    AN 109274-36-4  
              SOL    64-17-5 EtOH

RX(59) OF 107 COMPOSED OF RX(21), RX(29)  
RX(59)      AI    +    V    +    AE    ==>    AQ

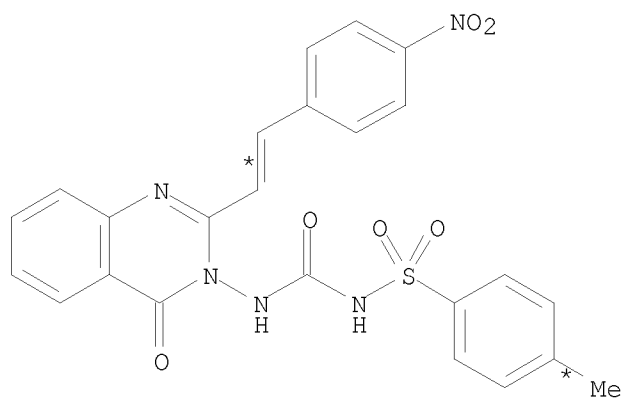


V



AE

2  
STEPS  
→



AQ  
YIELD 72%

RX(21)      RCT    AI 120-14-9, V 109274-28-4  
              RGT    M 64-19-7 AcOH  
              PRO    R 109274-27-3  
              SOL    64-17-5 EtOH

RX(29)      RCT    R 109274-27-3, AE 555-16-8

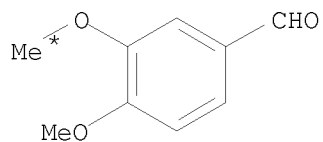


10/ 562,112

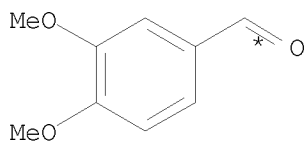
RGT M 64-19-7 AcOH  
PRO AQ 109274-37-5  
SOL 64-17-5 EtOH

RX(60) OF 107 COMPOSED OF RX(21), RX(31)

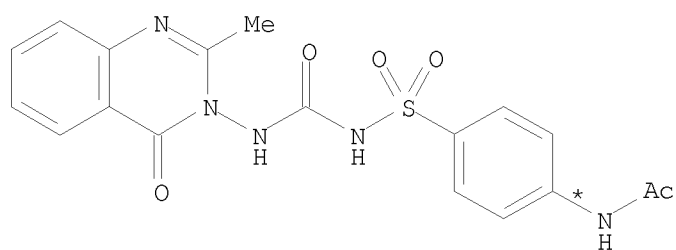
RX(60) 2 AI + V ==> AS



AI

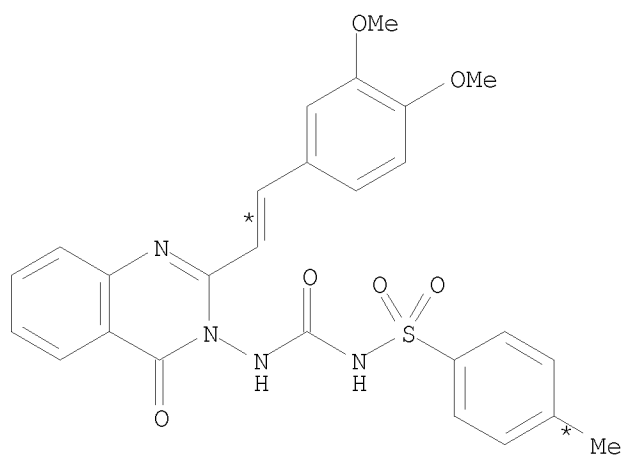


AI



V

2  
STEPS  
→



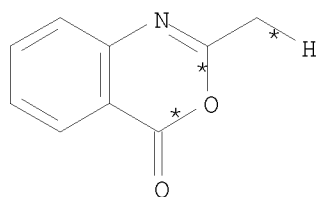
AS  
YIELD 58%

RX(21) RCT AI 120-14-9, V 109274-28-4  
RGT M 64-19-7 AcOH  
PRO R 109274-27-3  
SOL 64-17-5 EtOH

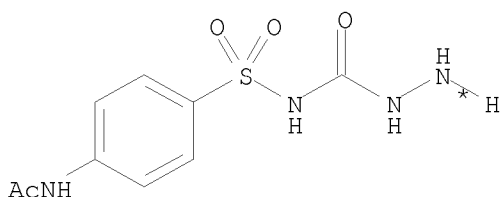
10/ 562,112

RX(31)      RCT   R 109274-27-3, AI 120-14-9  
              RGT   M 64-19-7 AcOH  
              PRO   AS 109274-38-6  
              SOL   64-17-5 EtOH

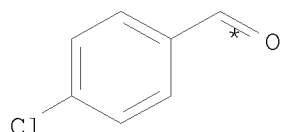
RX(66) OF 107 COMPOSED OF RX(12), RX(19)  
RX(66)      N + J + AC ==> AG



N

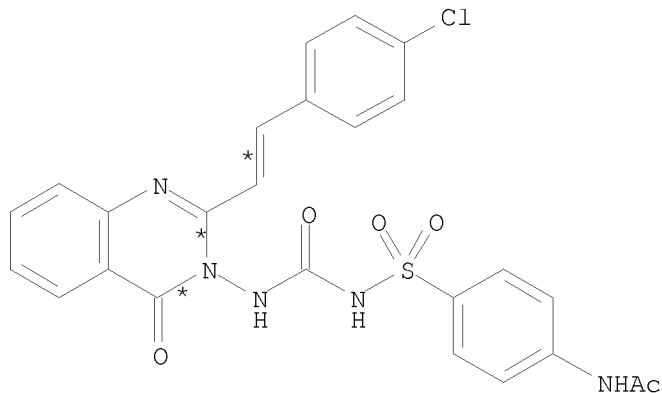


J



AC

2  
STEPS  
→



AG

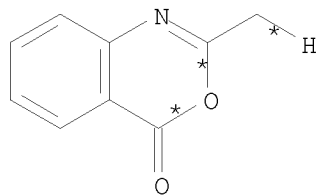
YIELD 84%

RX(12)      RCT   N 525-76-8, J 76983-56-7  
              PRO   V 109274-28-4  
              SOL   110-86-1 Pyridine

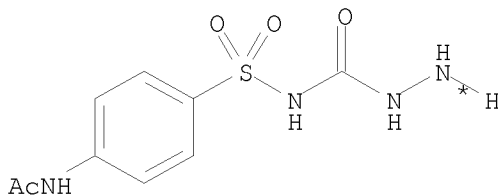
RX(19)      RCT   AC 104-88-1, V 109274-28-4  
              RGT   M 64-19-7 AcOH  
              PRO   AG 109274-46-6  
              SOL   64-17-5 EtOH

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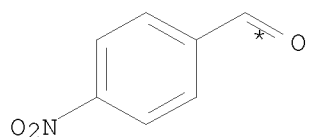
RX(67) OF 107 COMPOSED OF RX(12), RX(20)  
RX(67) N + J + AE ==> AH



N

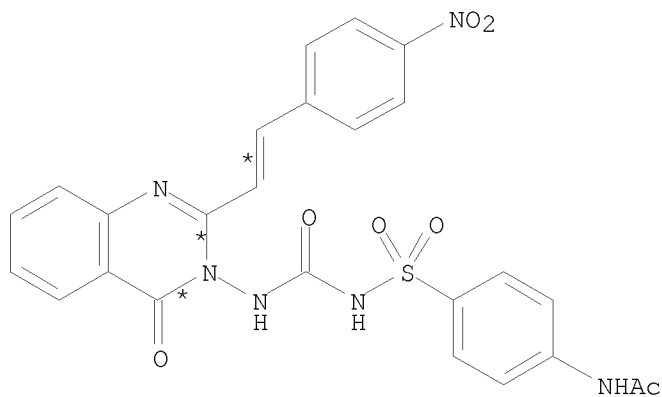


J



AE

2  
STEPS  
→



AH

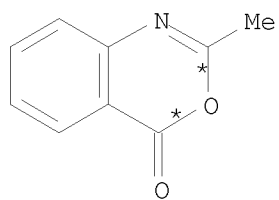
YIELD 76%

RX(12) RCT N 525-76-8, J 76983-56-7  
PRO V 109274-28-4  
SOL 110-86-1 Pyridine

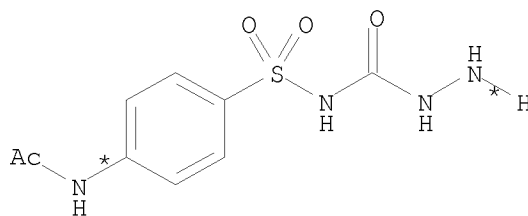
RX(20) RCT AE 555-16-8, V 109274-28-4  
RGT M 64-19-7 AcOH  
PRO AH 109274-47-7  
SOL 64-17-5 EtOH

RX(68) OF 107 COMPOSED OF RX(12), RX(21)  
RX(68) N + J + AI ==> R

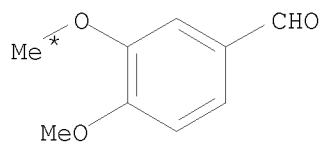
10/ 562,112



N

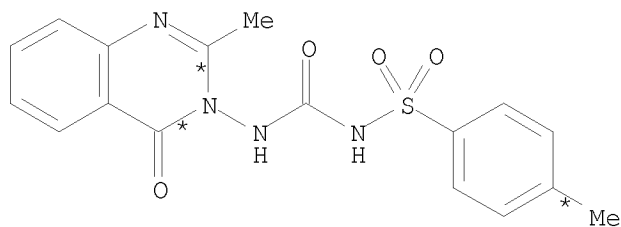


J



AI

2  
STEPS  
→



R

YIELD 82%

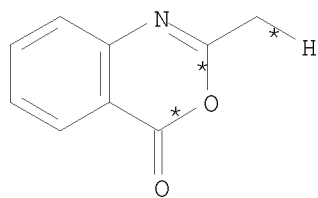
RX(12)      RCT   N 525-76-8, J 76983-56-7  
               PRO   V 109274-28-4  
               SOL   110-86-1 Pyridine

RX(21)      RCT   AI 120-14-9, V 109274-28-4  
               RGT   M 64-19-7 AcOH  
               PRO   R 109274-27-3  
               SOL   64-17-5 EtOH

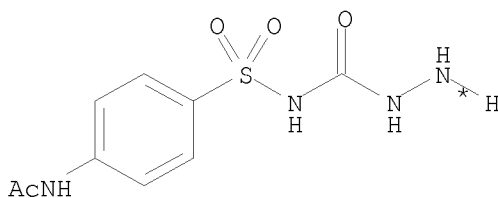
RX(69) OF 107 COMPOSED OF RX(12), RX(23)

RX(69)      N + J + W ==> AK

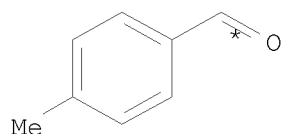
10/ 562,112



N

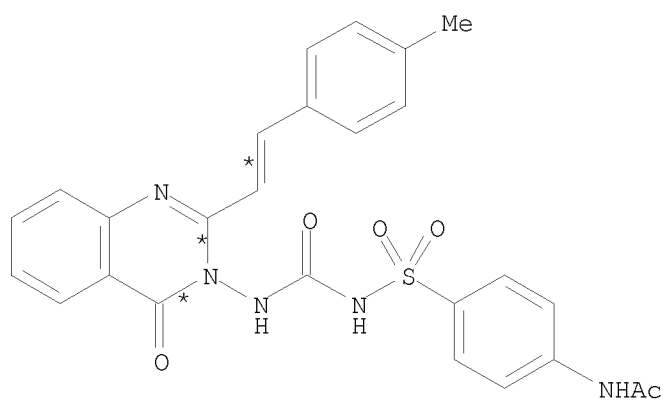


J



W

2  
STEPS  
→



AK

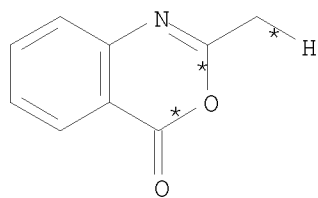
YIELD 86%

RX(12) RCT N 525-76-8, J 76983-56-7  
PRO V 109274-28-4  
SOL 110-86-1 Pyridine

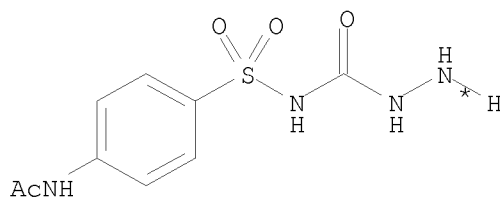
RX(23) RCT V 109274-28-4, W 104-87-0  
RGT M 64-19-7 AcOH  
PRO AK 109274-44-4  
SOL 64-17-5 EtOH

RX(70) OF 107 COMPOSED OF RX(12), RX(25)  
RX(70) N + J + Y ==> AM

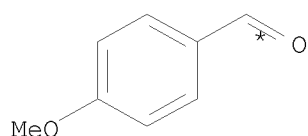
10/ 562,112



N

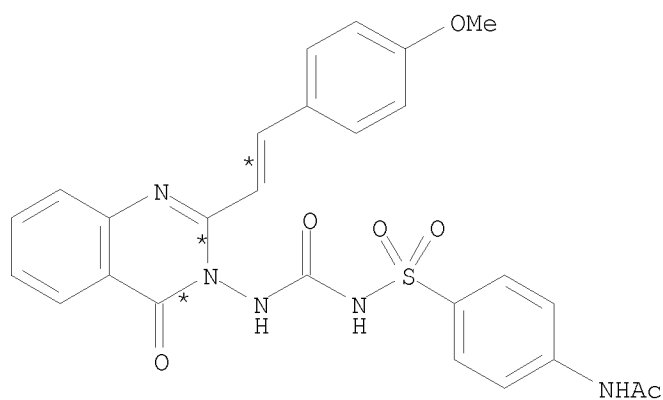


J



Y

2  
STEPS  
→



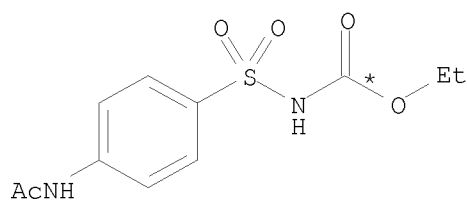
AM

YIELD 76%

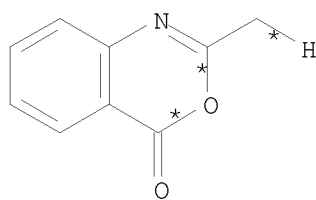
RX(12) RCT N 525-76-8, J 76983-56-7  
PRO V 109274-28-4  
SOL 110-86-1 Pyridine

RX(25) RCT V 109274-28-4, Y 123-11-5  
RGT M 64-19-7 AcOH  
PRO AM 109274-45-5  
SOL 64-17-5 EtOH

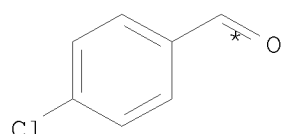
RX(90) OF 107 COMPOSED OF RX(4), RX(12), RX(19)  
RX(90) I + N + AC ==> AG



I

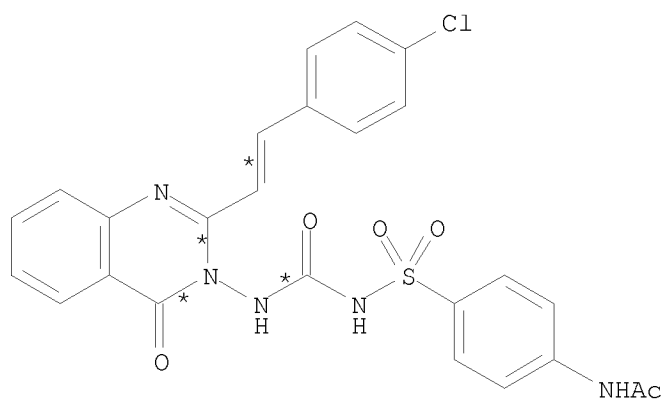


N



AC

3  
STEPS  
→



AG

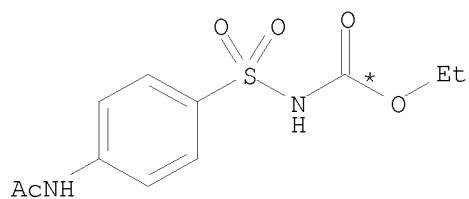
YIELD 84%

RX(4)	RCT	I 13945-59-0
	RGT	C 302-01-2 N <sub>2</sub> H <sub>4</sub>
	PRO	J 76983-56-7
	SOL	64-17-5 EtOH
RX(12)	RCT	N 525-76-8, J 76983-56-7
	PRO	V 109274-28-4
	SOL	110-86-1 Pyridine
RX(19)	RCT	AC 104-88-1, V 109274-28-4
	RGT	M 64-19-7 AcOH
	PRO	AG 109274-46-6
	SOL	64-17-5 EtOH

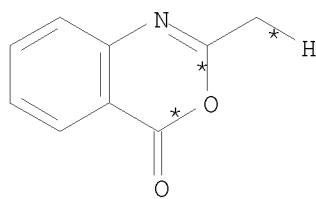
RX(91) OF 107 COMPOSED OF RX(4), RX(12), RX(20)

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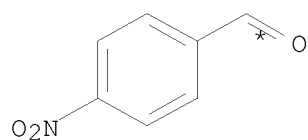
RX(91)      I   +   N   +   AE   ==>   AH



I

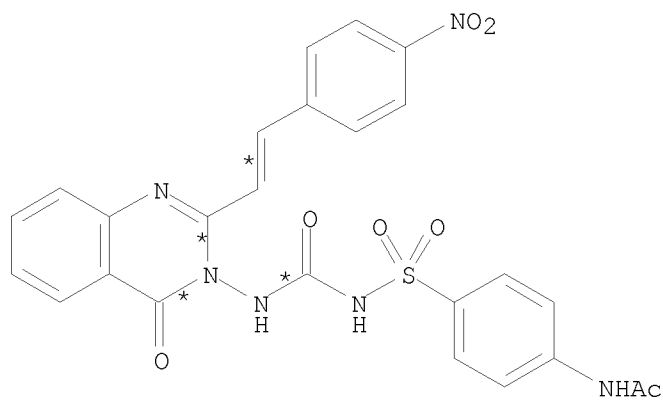


N



AE

3  
STEPS  
→



AH

YIELD 76%

RX(4)      RCT   I 13945-59-0  
             RGT   C 302-01-2 N<sub>2</sub>H<sub>4</sub>  
             PRO   J 76983-56-7  
             SOL   64-17-5 EtOH

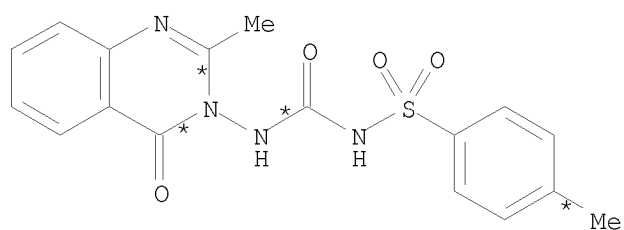
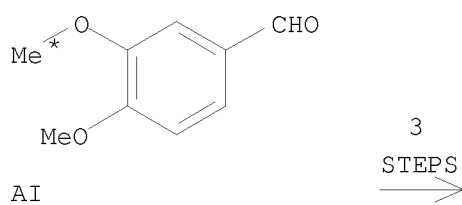
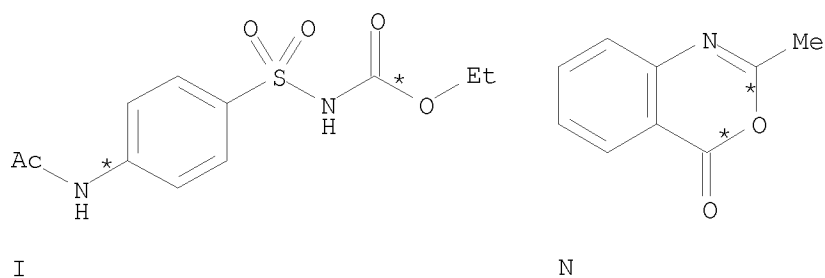
RX(12)     RCT   N 525-76-8, J 76983-56-7  
             PRO   V 109274-28-4  
             SOL   110-86-1 Pyridine

RX(20)     RCT   AE 555-16-8, V 109274-28-4  
             RGT   M 64-19-7 AcOH  
             PRO   AH 109274-47-7  
             SOL   64-17-5 EtOH



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RX(92) OF 107 COMPOSED OF RX(4), RX(12), RX(21)  
RX(92) I + N + AI ==> R

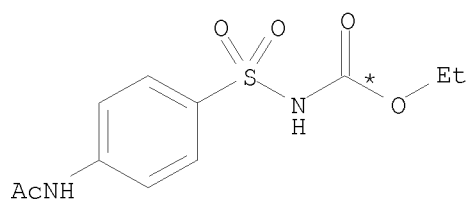


R  
YIELD 82%

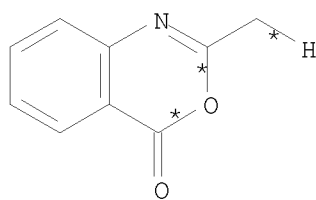
RX(4)	RCT	I 13945-59-0
	RGT	C 302-01-2 N <sub>2</sub> H <sub>4</sub>
	PRO	J 76983-56-7
	SOL	64-17-5 EtOH
RX(12)	RCT	N 525-76-8, J 76983-56-7
	PRO	V 109274-28-4
	SOL	110-86-1 Pyridine
RX(21)	RCT	AI 120-14-9, V 109274-28-4
	RGT	M 64-19-7 AcOH
	PRO	R 109274-27-3
	SOL	64-17-5 EtOH

RX(93) OF 107 COMPOSED OF RX(4), RX(12), RX(23)  
RX(93) I + N + W ==> AK

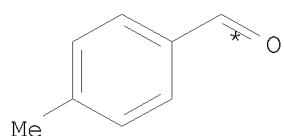
10/ 562,112



I

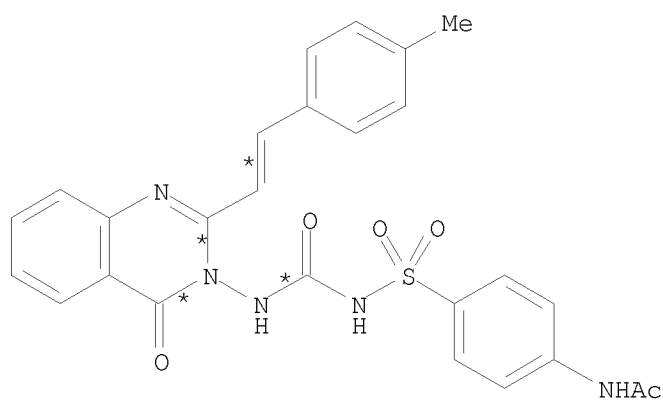


N



W

3  
STEPS  
→



AK

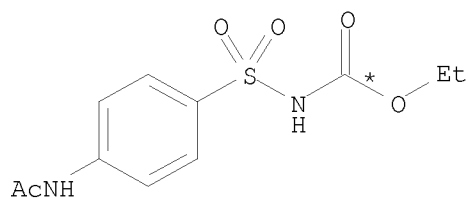
YIELD 86%

RX(4)	RCT	I 13945-59-0
	RGT	C 302-01-2 N2H4
	PRO	J 76983-56-7
	SOL	64-17-5 EtOH
RX(12)	RCT	N 525-76-8, J 76983-56-7
	PRO	V 109274-28-4
	SOL	110-86-1 Pyridine
RX(23)	RCT	V 109274-28-4, W 104-87-0
	RGT	M 64-19-7 AcOH
	PRO	AK 109274-44-4
	SOL	64-17-5 EtOH

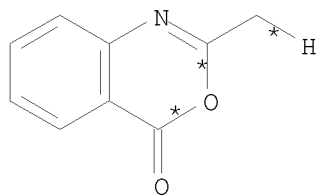
RX(94) OF 107 COMPOSED OF RX(4), RX(12), RX(25)

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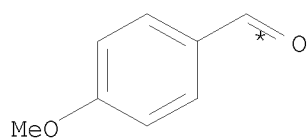
RX(94)      I   +   N   +   Y   ==>   AM



I

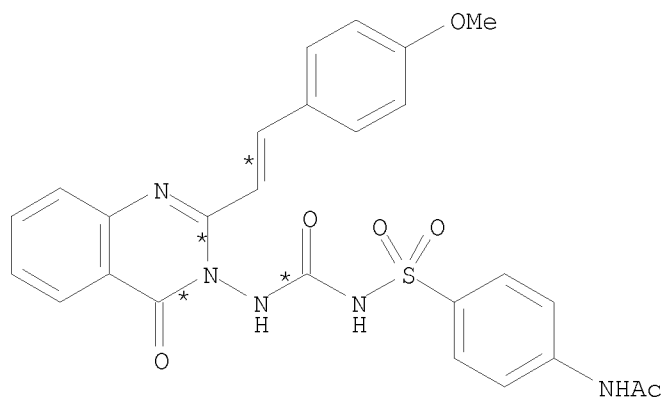


N



Y

3  
STEPS  
→



AM

YIELD 76%

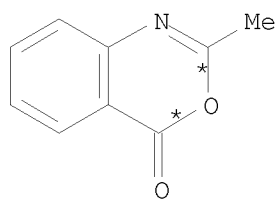
RX(4)      RCT    I 13945-59-0  
              RGT    C 302-01-2 N<sub>2</sub>H<sub>4</sub>  
              PRO    J 76983-56-7  
              SOL    64-17-5 EtOH

RX(12)     RCT    N 525-76-8, J 76983-56-7  
              PRO    V 109274-28-4  
              SOL    110-86-1 Pyridine

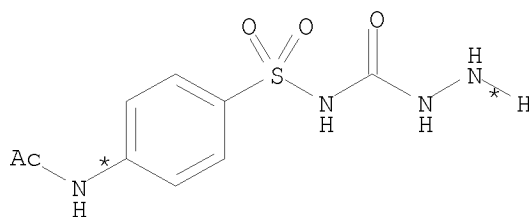
RX(25)     RCT    V 109274-28-4, Y 123-11-5  
              RGT    M 64-19-7 AcOH  
              PRO    AM 109274-45-5  
              SOL    64-17-5 EtOH

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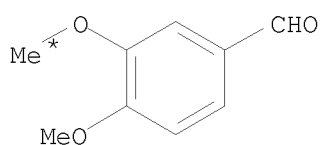
RX(95) OF 107 COMPOSED OF RX(12), RX(21), RX(15)  
RX(95) N + J + AI + W ==> AA



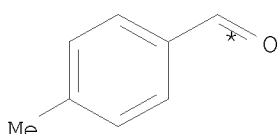
N



J

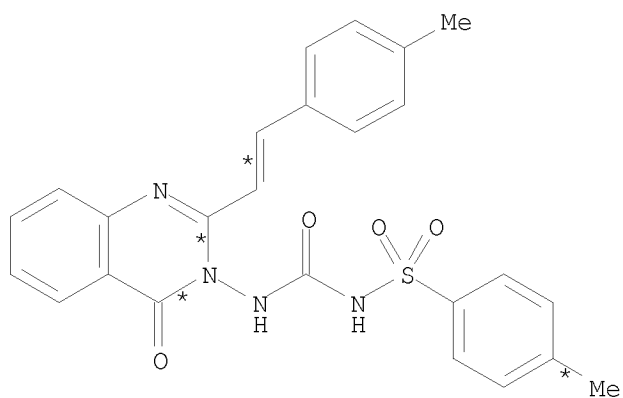


AI



W

3  
STEPS  
→



AA

YIELD 54%

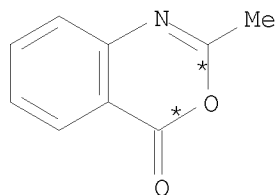
RX(12) RCT N 525-76-8, J 76983-56-7  
PRO V 109274-28-4  
SOL 110-86-1 Pyridine

RX(21) RCT AI 120-14-9, V 109274-28-4  
RGT M 64-19-7 AcOH  
PRO R 109274-27-3  
SOL 64-17-5 EtOH

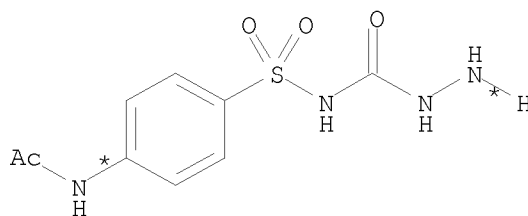
RX(15) RCT W 104-87-0, R 109274-27-3  
RGT M 64-19-7 AcOH  
PRO AA 109274-34-2  
SOL 64-17-5 EtOH

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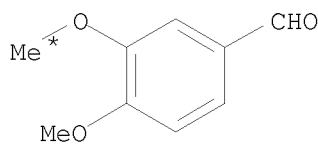
RX(96) OF 107 COMPOSED OF RX(12), RX(21), RX(16)  
RX(96) N + J + AI + Y ==> AB



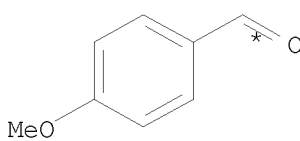
N



J

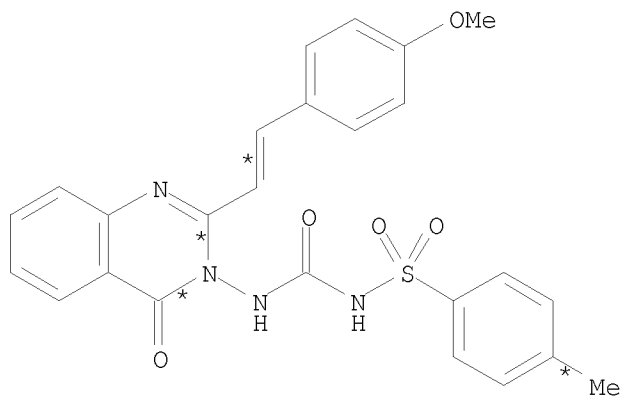


AI



Y

3  
STEPS  
→



AB

YIELD 60%

RX(12) RCT N 525-76-8, J 76983-56-7  
PRO V 109274-28-4  
SOL 110-86-1 Pyridine

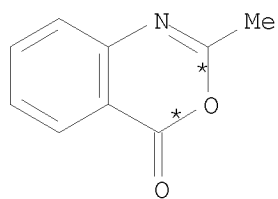
RX(21) RCT AI 120-14-9, V 109274-28-4  
RGT M 64-19-7 AcOH  
PRO R 109274-27-3  
SOL 64-17-5 EtOH

RX(16) RCT Y 123-11-5, R 109274-27-3  
RGT M 64-19-7 AcOH

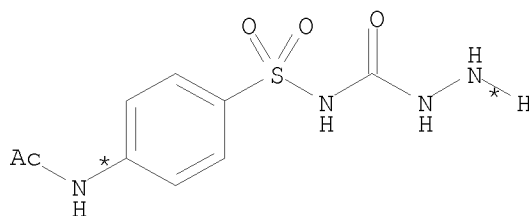
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PRO AB 109274-35-3  
SOL 64-17-5 EtOH

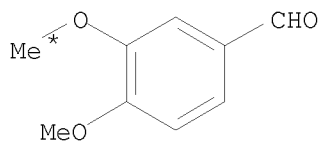
RX(97) OF 107 COMPOSED OF RX(12), RX(21), RX(26)  
RX(97) N + J + AI + AC ==> AN



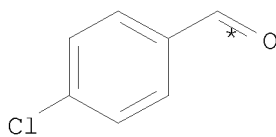
N



J

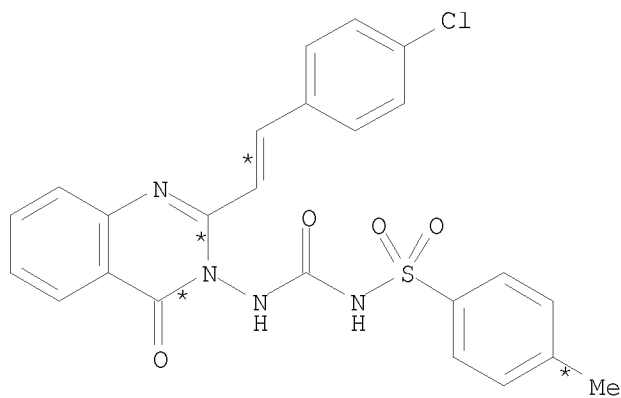


AI



AC

3  
STEPS  
→



AN

YIELD 68%

RX(12) RCT N 525-76-8, J 76983-56-7  
PRO V 109274-28-4  
SOL 110-86-1 Pyridine

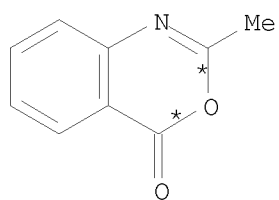
RX(21) RCT AI 120-14-9, V 109274-28-4  
RGT M 64-19-7 AcOH  
PRO R 109274-27-3  
SOL 64-17-5 EtOH

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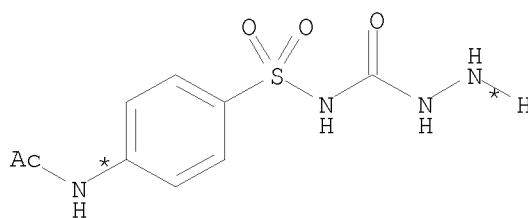
RX(26) RCT R 109274-27-3, AC 104-88-1  
RGT M 64-19-7 AcOH  
PRO AN 109274-36-4  
SOL 64-17-5 EtOH

RX(98) OF 107 COMPOSED OF RX(12), RX(21), RX(29)

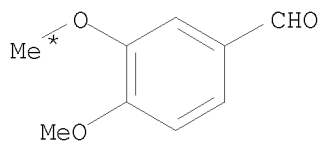
RX(98) N + J + AI + AE ==> AQ



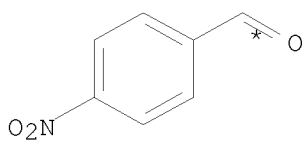
N



J

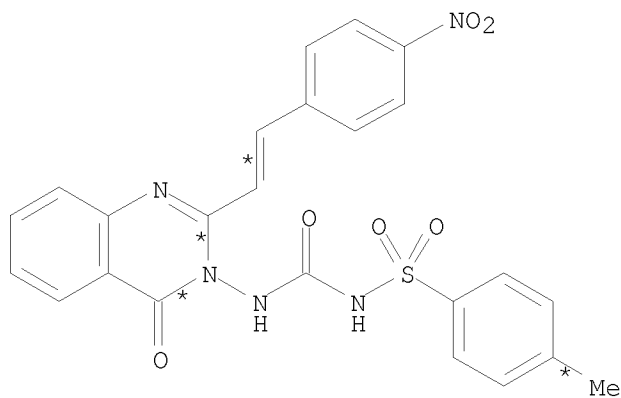


AI



AE

3  
STEPS  
→



AQ

YIELD 72%

RX(12) RCT N 525-76-8, J 76983-56-7  
PRO V 109274-28-4  
SOL 110-86-1 Pyridine

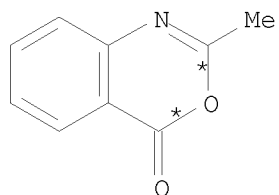
RX(21) RCT AI 120-14-9, V 109274-28-4  
RGT M 64-19-7 AcOH  
PRO R 109274-27-3

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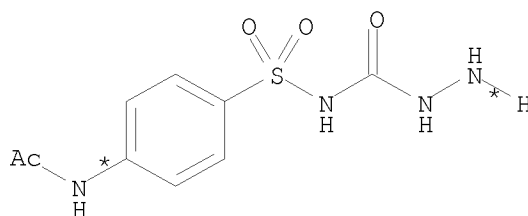
SOL 64-17-5 EtOH

RX(29) RCT R 109274-27-3, AE 555-16-8  
RGT M 64-19-7 AcOH  
PRO AQ 109274-37-5  
SOL 64-17-5 EtOH

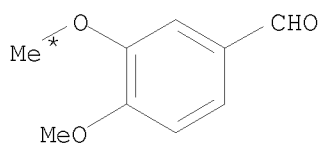
RX(99) OF 107 COMPOSED OF RX(12), RX(21), RX(31)  
RX(99) N + J + 2 AI ==> AS



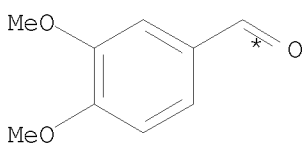
N



J

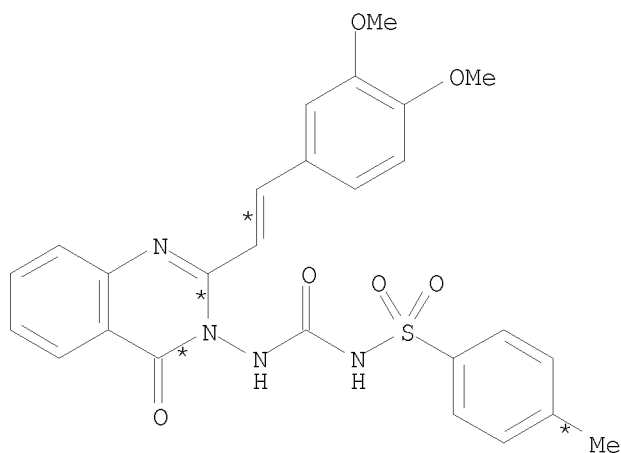


AI



AI

3  
STEPS  
→



AS  
YIELD 58%

RX(12) RCT N 525-76-8, J 76983-56-7  
PRO V 109274-28-4  
SOL 110-86-1 Pyridine

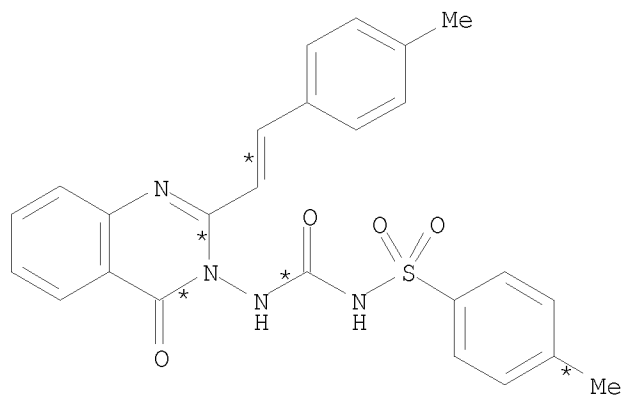
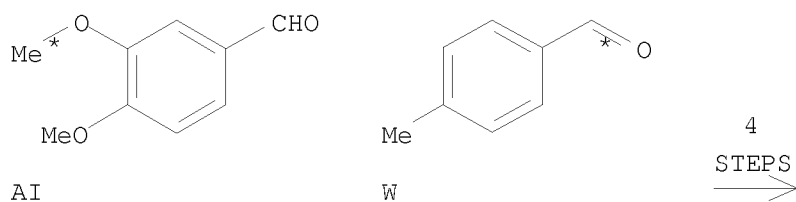
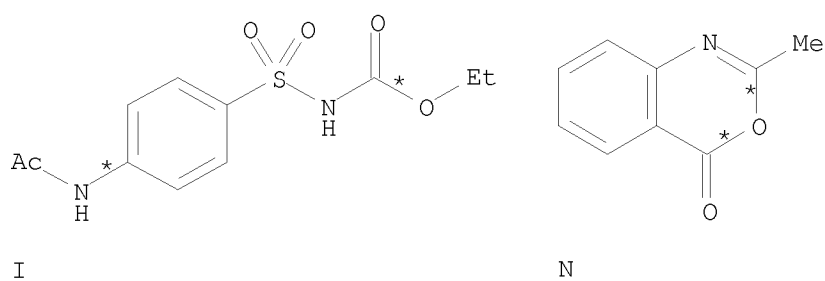


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RX(21) RCT AI 120-14-9, V 109274-28-4  
RGT M 64-19-7 AcOH  
PRO R 109274-27-3  
SOL 64-17-5 EtOH

RX(31) RCT R 109274-27-3, AI 120-14-9  
RGT M 64-19-7 AcOH  
PRO AS 109274-38-6  
SOL 64-17-5 EtOH

RX(100) OF 107 COMPOSED OF RX(4), RX(12), RX(21), RX(15)  
RX(100) I + N + AI + W ==> AA



AA  
YIELD 54%

RX(4) RCT I 13945-59-0

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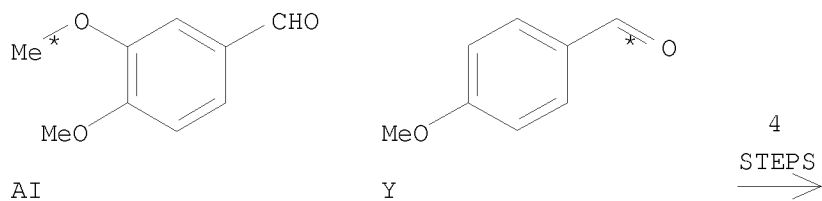
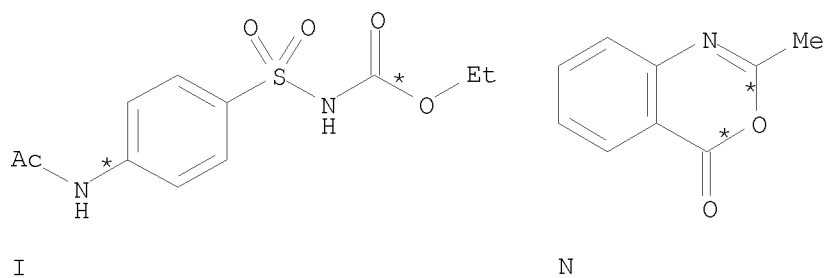
RGT C 302-01-2 N2H4  
PRO J 76983-56-7  
SOL 64-17-5 EtOH

RX(12) RCT N 525-76-8, J 76983-56-7  
PRO V 109274-28-4  
SOL 110-86-1 Pyridine

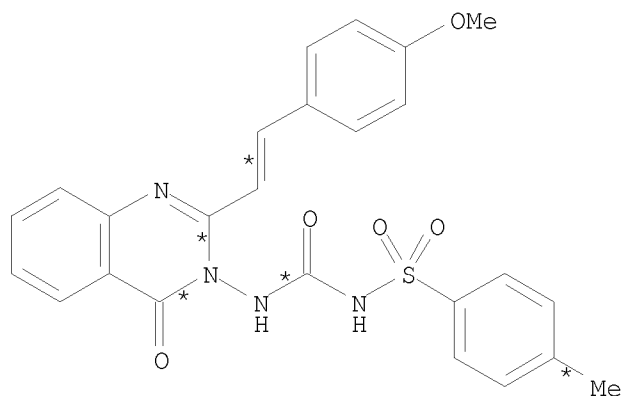
RX(21) RCT AI 120-14-9, V 109274-28-4  
RGT M 64-19-7 AcOH  
PRO R 109274-27-3  
SOL 64-17-5 EtOH

RX(15) RCT W 104-87-0, R 109274-27-3  
RGT M 64-19-7 AcOH  
PRO AA 109274-34-2  
SOL 64-17-5 EtOH

RX(101) OF 107 COMPOSED OF RX(4), RX(12), RX(21), RX(16)  
RX(101) I + N + AI + Y ==> AB



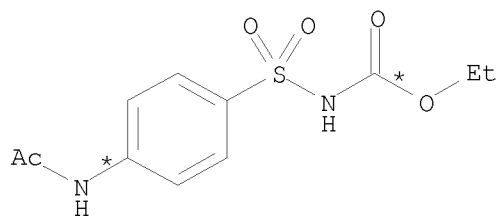
10/ 562,112



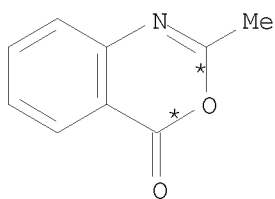
AB  
YIELD 60%

RX(4)	RCT	I 13945-59-0
	RGT	C 302-01-2 N <sub>2</sub> H <sub>4</sub>
	PRO	J 76983-56-7
	SOL	64-17-5 EtOH
RX(12)	RCT	N 525-76-8, J 76983-56-7
	PRO	V 109274-28-4
	SOL	110-86-1 Pyridine
RX(21)	RCT	AI 120-14-9, V 109274-28-4
	RGT	M 64-19-7 AcOH
	PRO	R 109274-27-3
	SOL	64-17-5 EtOH
RX(16)	RCT	Y 123-11-5, R 109274-27-3
	RGT	M 64-19-7 AcOH
	PRO	AB 109274-35-3
	SOL	64-17-5 EtOH

RX(102) OF 107 COMPOSED OF RX(4), RX(12), RX(21), RX(26)  
RX(102) I + N + AI + AC ==> AN

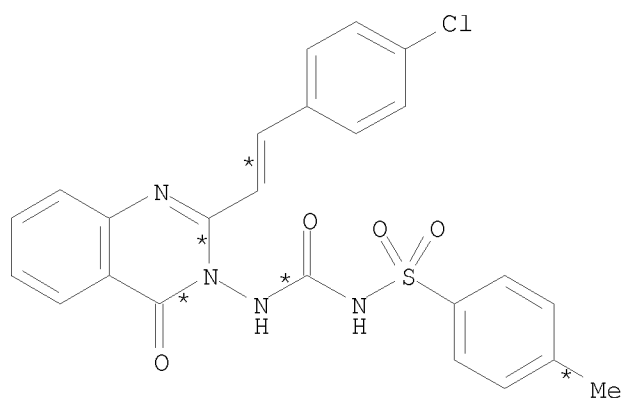
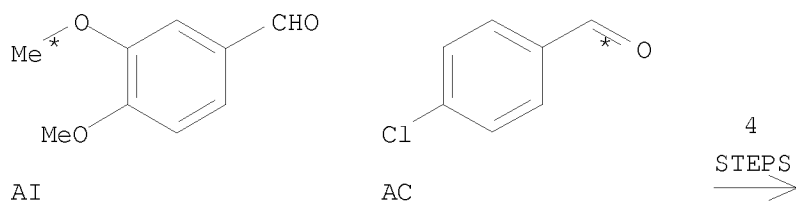


I



N

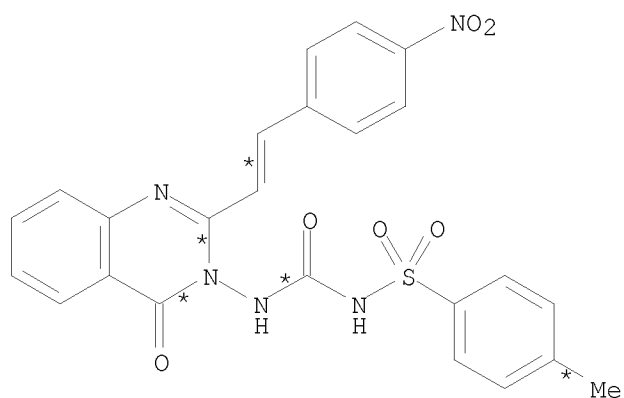
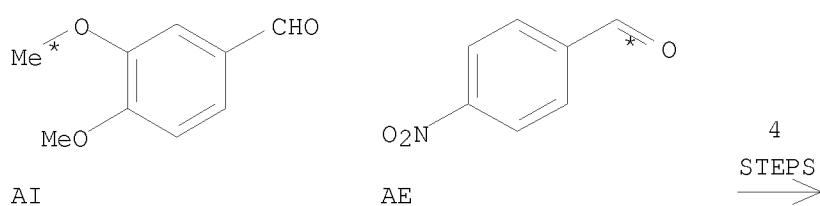
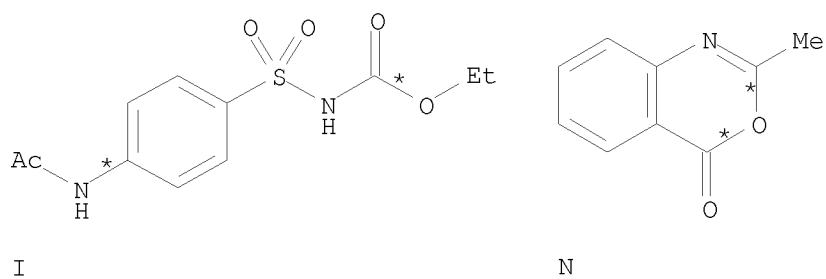
10/ 562,112



AN  
YIELD 68%

RX(4)	RCT	I 13945-59-0
	RGT	C 302-01-2 N <sub>2</sub> H <sub>4</sub>
	PRO	J 76983-56-7
	SOL	64-17-5 EtOH
RX(12)	RCT	N 525-76-8, J 76983-56-7
	PRO	V 109274-28-4
	SOL	110-86-1 Pyridine
RX(21)	RCT	AI 120-14-9, V 109274-28-4
	RGT	M 64-19-7 AcOH
	PRO	R 109274-27-3
	SOL	64-17-5 EtOH
RX(26)	RCT	R 109274-27-3, AC 104-88-1
	RGT	M 64-19-7 AcOH
	PRO	AN 109274-36-4
	SOL	64-17-5 EtOH

RX(103) OF 107 COMPOSED OF RX(4), RX(12), RX(21), RX(29)  
 RX(103) I + N + AI + AE ==> AQ



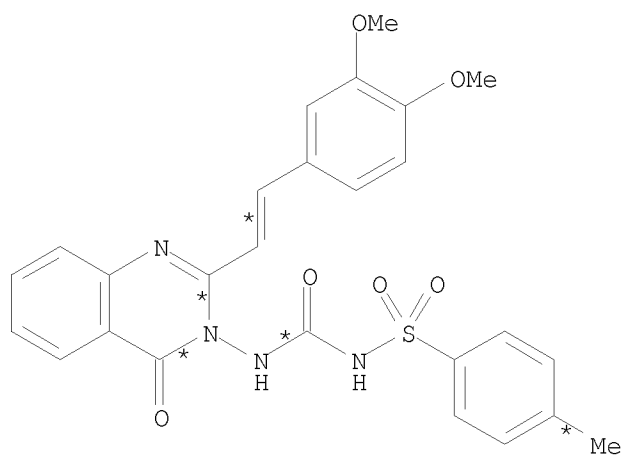
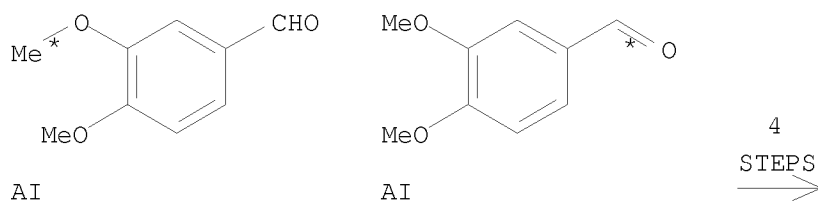
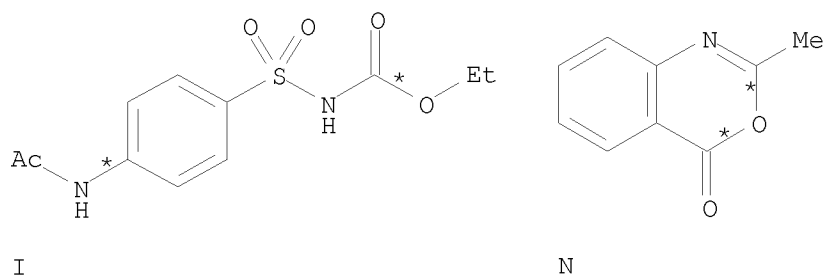
YIELD 72%

RX(4)	RCT	I 13945-59-0
	RGT	C 302-01-2 N <sub>2</sub> H <sub>4</sub>
	PRO	J 76983-56-7
	SOL	64-17-5 EtOH
RX(12)	RCT	N 525-76-8, J 76983-56-7
	PRO	V 109274-28-4
	SOL	110-86-1 Pyridine
RX(21)	RCT	AI 120-14-9, V 109274-28-4
	RGT	M 64-19-7 AcOH
	PRO	R 109274-27-3
	SOL	64-17-5 EtOH

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RX(29) RCT R 109274-27-3, AE 555-16-8  
RGT M 64-19-7 AcOH  
PRO AQ 109274-37-5  
SOL 64-17-5 EtOH

RX(104) OF 107 COMPOSED OF RX(4), RX(12), RX(21), RX(31)  
RX(104) I + N + 2 AI ==> AS



YIELD 58%

RX(4) RCT I 13945-59-0  
RGT C 302-01-2 N2H4  
PRO J 76983-56-7  
SOL 64-17-5 EtOH

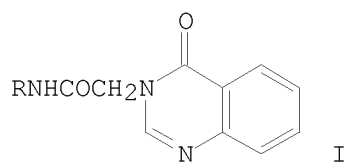
10/ 562,112

RX(12) RCT N 525-76-8, J 76983-56-7  
PRO V 109274-28-4  
SOL 110-86-1 Pyridine

RX(21) RCT AI 120-14-9, V 109274-28-4  
RGT M 64-19-7 AcOH  
PRO R 109274-27-3  
SOL 64-17-5 EtOH

RX(31) RCT R 109274-27-3, AI 120-14-9  
RGT M 64-19-7 AcOH  
PRO AS 109274-38-6  
SOL 64-17-5 EtOH

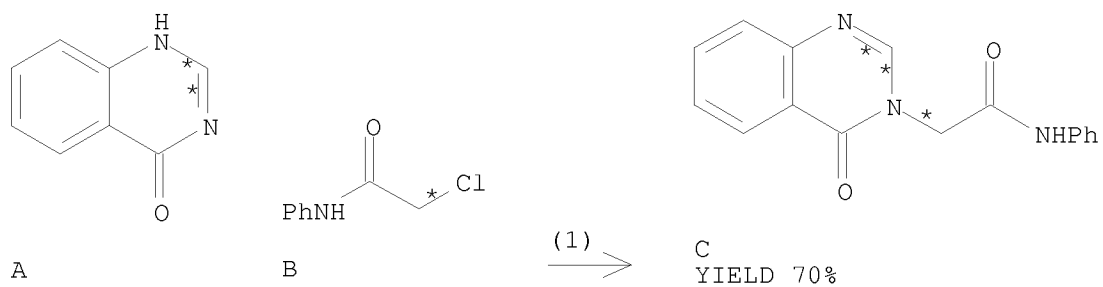
L3 ANSWER 184 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 106:196363 CASREACT  
TITLE: Monoamine oxidase and succinate dehydrogenase  
inhibitory and anticonvulsant activities of some  
3-(N-arylcarbamoylmethyl)-4-quinazolones  
AUTHOR(S): Saksena, R. K.; Yasmeen, Rana, Ms.  
CORPORATE SOURCE: D.A.V. Coll., Kanpur Univ., Kanpur, 208 001, India  
SOURCE: Indian Journal of Chemistry, Section B: Organic  
Chemistry Including Medicinal Chemistry (1986),  
25B(4), 438-40  
CODEN: IJSBDB; ISSN: 0376-4699  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB 3-(N-Arylcarbamoylmethyl)-4-quinazolones I (R = Ph, substituted phenyl)  
(11 compds.) were prepared from RNHCOCH<sub>2</sub>Cl and 4-quinazolinone. I have ALD<sub>50</sub>  
values from 500-1000 mg/kg and inhibit rat brain monoamine oxidase  
(30-65%) and succinate dehydrogenase (10-80%) in vitro at a concentration of 5  
+ 10<sup>-4</sup> M and provide 30-50% protection against  
pentylenetetrazole-induced convulsions in mice.

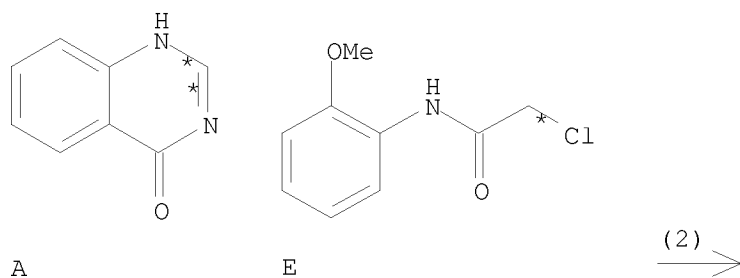
RX(1) OF 33 ...A + B ==> C

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RX(1) RCT A 491-36-1, B 587-65-5  
PRO C 108086-38-0  
SOL 110-86-1 Pyridine

RX(2) OF 33 ...A + E ==> F



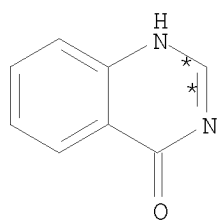
F  
YIELD 60%

RX(2) RCT A 491-36-1, E 55860-22-5  
PRO F 108086-39-1  
SOL 110-86-1 Pyridine

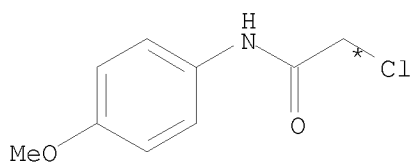
RX(3) OF 33 ...A + G ==> H



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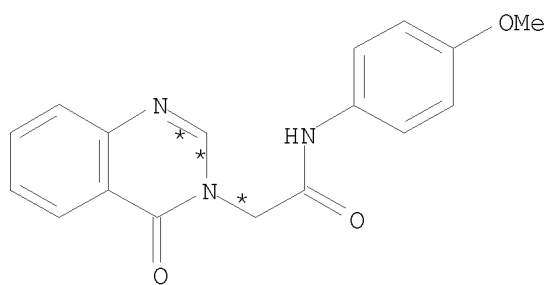


A



G

(3)  $\longrightarrow$

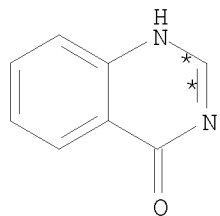


H

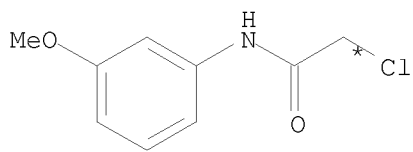
YIELD 65%

RX(3) RCT A 491-36-1, G 22303-36-2  
PRO H 108086-40-4  
SOL 110-86-1 Pyridine

RX(4) OF 33 ...A + I ==> J



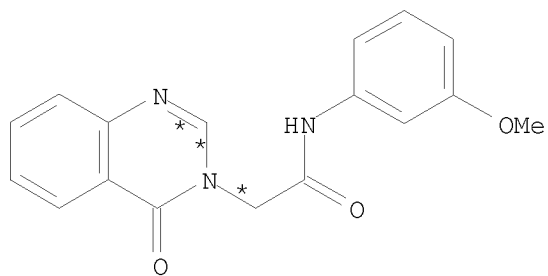
A



I

(4)  $\longrightarrow$

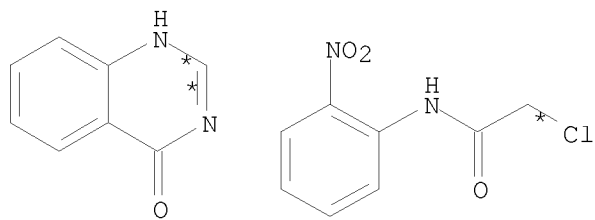
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J  
YIELD 75%

RX(4) RCT A 491-36-1, I 17641-08-6  
PRO J 108086-41-5  
SOL 110-86-1 Pyridine

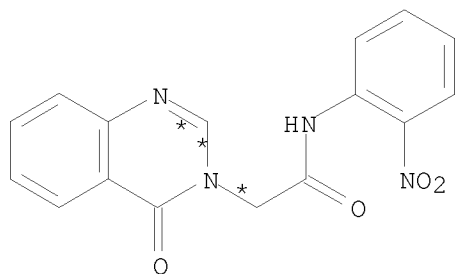
RX(5) OF 33 ...A + K ==> L



A

K

(5)  $\longrightarrow$

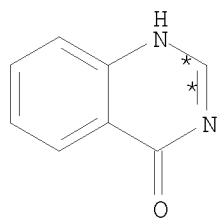


L  
YIELD 70%

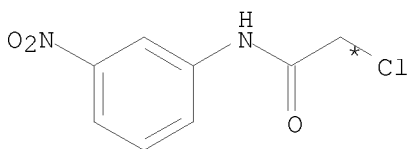
RX(5) RCT A 491-36-1, K 10147-70-3  
PRO L 108086-42-6  
SOL 110-86-1 Pyridine

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RX(6) OF 33      ...A + M ==> N

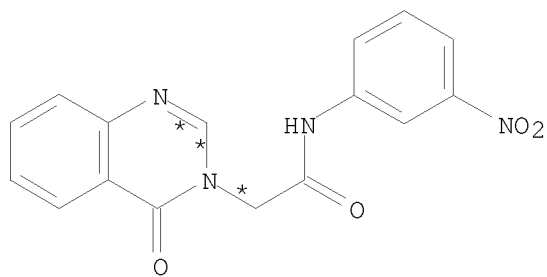


A



M

(6)  $\longrightarrow$

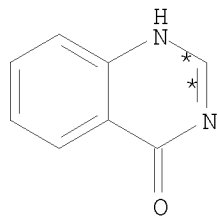


N

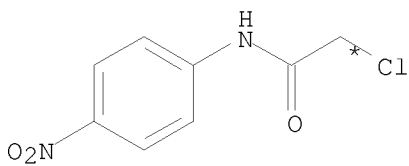
YIELD 60%

RX(6)      RCT    A 491-36-1, M 10147-71-4  
             PRO    N 108086-43-7  
             SOL    110-86-1 Pyridine

RX(7) OF 33      ...A + O ==> P



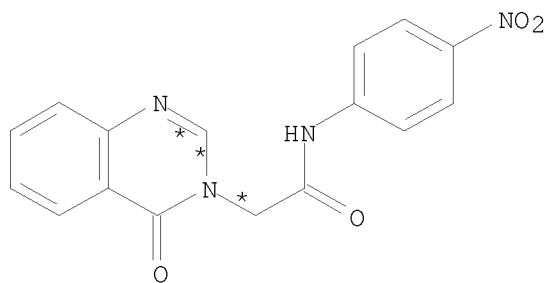
A



O

(7)  $\longrightarrow$

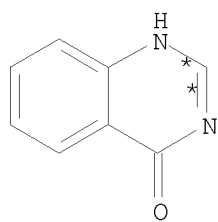
10/ 562,112



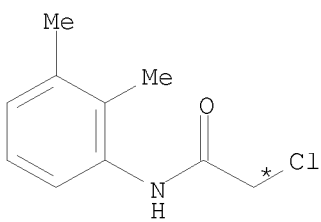
P  
YIELD 65%

RX(7) RCT A 491-36-1, O 17329-87-2  
PRO P 108086-44-8  
SOL 110-86-1 Pyridine

RX(8) OF 33 ...A + Q ==> R

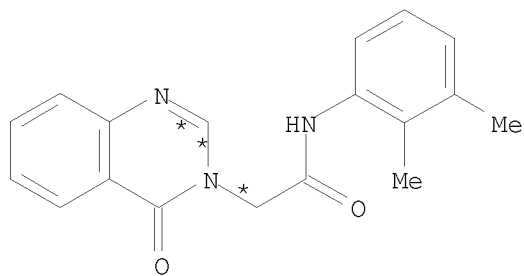


A



Q

(8)  $\longrightarrow$

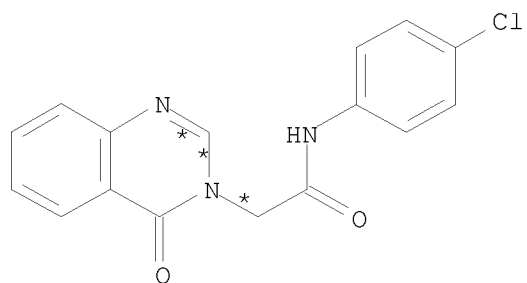
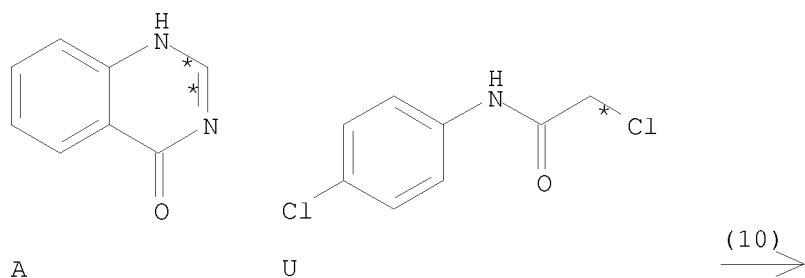


R  
YIELD 68%

RX(8) RCT A 491-36-1, Q 2564-07-0  
PRO R 108086-45-9  
SOL 110-86-1 Pyridine

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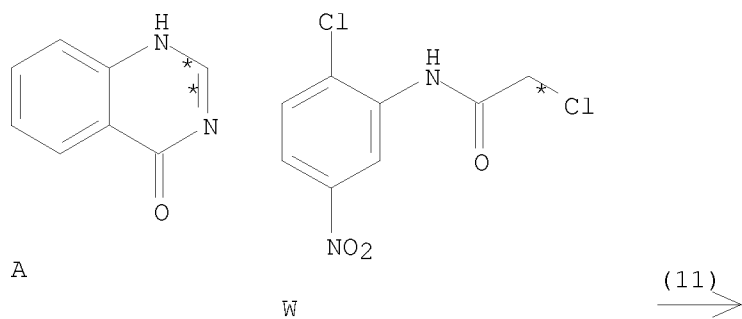
RX(10) OF 33      ...A + U ==> V



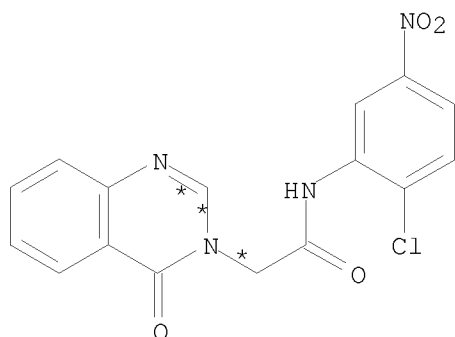
V  
YIELD 70%

RX(10)      RCT    A 491-36-1, U 3289-75-6  
              PRO    V 108086-47-1  
              SOL    110-86-1 Pyridine

RX(11) OF 33      ...A + W ==> X

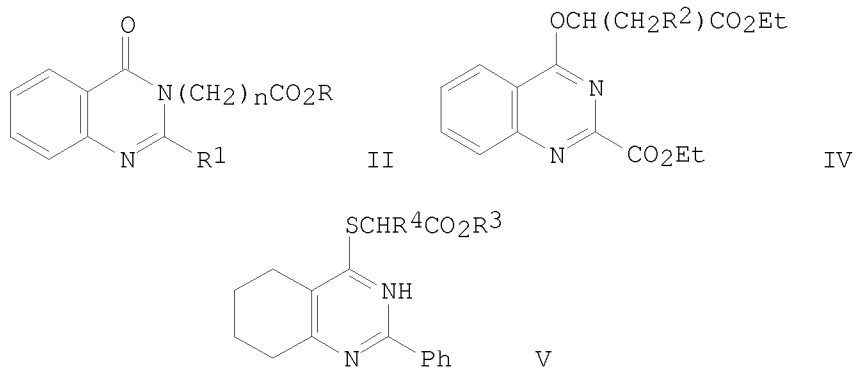


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RX(11) RCT A 491-36-1, W 108086-37-9  
PRO X 108086-48-2  
SOL 110-86-1 Pyridine

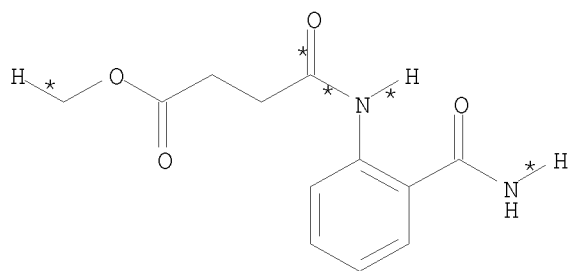
L3 ANSWER 185 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 106:138387 CASREACT  
TITLE: Quinazolinecarboxylic acid. Synthesis of  
alkyl[2-(ethoxycarbonyl)-3,4-dihydro-4-oxoquinazolin-3-yl]-, [2-(ethoxycarbonyl)quinazolin-4-yloxy]- and (5,6,7,8-tetrahydro-2-phenylquinazolin-4-ylthio)alkanoates  
AUTHOR(S): Suesse, Manfred; Adler, Frank; Johne, Siegfried  
CORPORATE SOURCE: Inst. Biochem. Pflanzen Halle, Dtsch. Akad. Wiss., Halle/Saale, DDR-4010, Ger. Dem. Rep.  
SOURCE: Helvetica Chimica Acta (1986), 69(5), 1017-24  
CODEN: HCACAV; ISSN: 0018-019X  
DOCUMENT TYPE: Journal  
LANGUAGE: German  
GI



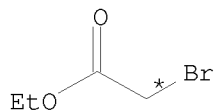
10/ 562,112

AB Cyclization of 2-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CONH(CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>Et (I, n = 2, 3) with EtO<sub>2</sub>CCO<sub>2</sub>Et gave quinazolines II (R = Et, R<sub>1</sub> = CO<sub>2</sub>Et), whereas, condensation of I (n = 1) with ClCOC<sub>2</sub>OEt gave a mixture of 2-EtO<sub>2</sub>CCONHC<sub>6</sub>H<sub>4</sub>CONHCH<sub>2</sub>CO<sub>2</sub>Et and II (n = 1, R = Et, R<sub>1</sub> = CO<sub>2</sub>Et). Cyclization of 2-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CONH<sub>2</sub> (III) with EtO<sub>2</sub>CCO<sub>2</sub>Et followed by condensation with BrCH<sub>2</sub>CO<sub>2</sub>R (R = Me, Et) gave II (n = 1, R = Me, Et, R<sub>1</sub> = CO<sub>2</sub>Et), whereas, cyclization of III with EtO<sub>2</sub>CCO<sub>2</sub>Et followed by condensation with R<sub>2</sub>CH<sub>2</sub>CHBrCO<sub>2</sub>Et (R<sub>2</sub> = H, Me) gave quinazoline esters IV. Condensation of III with ClCOCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>Me gave 2-H<sub>2</sub>NCOC<sub>6</sub>H<sub>4</sub>NHCOCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>Me which was cyclized with BrCH<sub>2</sub>CO<sub>2</sub>Et to give II (n = 1, R = Et, R<sub>1</sub> = CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>Et). Quinazoline thioethers V (R<sub>3</sub> = Me, Et, R<sub>4</sub> = H, Et, CHMe<sub>2</sub>) were prepared by aminolysis of 5,6,7,8-tetrahydro-1,3-benzoxazine-4(3H)-thione followed by condensation with BrCHR<sub>4</sub>CO<sub>2</sub>R<sub>3</sub>.

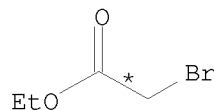
RX(11) OF 27 ...AC + 2 AD ==> AE



AC

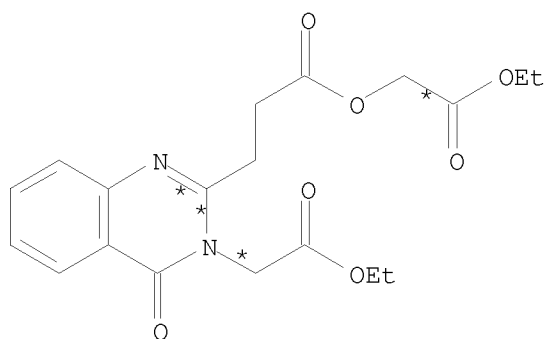


AD



AD

(11) →



AE  
YIELD 22%

RX(11) RCT AC 105234-41-1

STAGE(1)

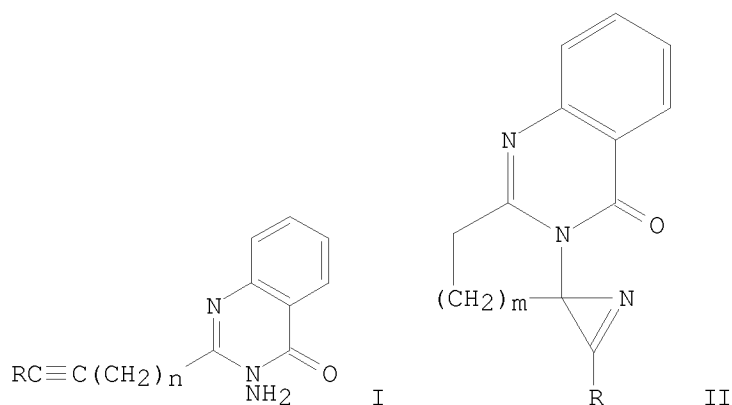
RGT P 7646-69-7 NaH

SOL 67-68-5 DMSO

STAGE(2)  
 RCT AD 105-36-2

PRO AE 105234-42-2

L3 ANSWER 186 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 106:138380 CASREACT  
 TITLE: Intramolecular reactions of N-nitrenes with alkynes:  
 conformational anchoring in spiro-fused 2H-azirines  
 AUTHOR(S): Atkinson, Robert S.; Grimshire, Michael J.  
 CORPORATE SOURCE: Dep. Chem., Univ. Leicester, Leicester, LE1 7RH, UK  
 SOURCE: Journal of the Chemical Society, Perkin Transactions  
 1: Organic and Bio-Organic Chemistry (1972-1999)  
 (1986), (7), 1215-24  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

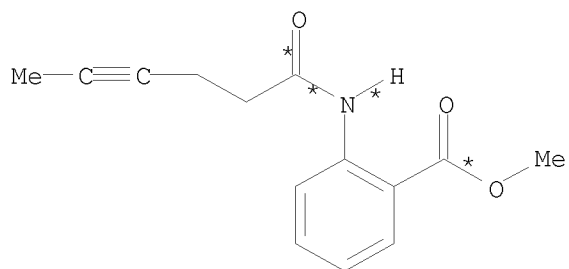


AB Oxidation of aminoquinazolinones, e.g., I ( $n = 2$ ,  $R = H$ , Me;  $n = 3$ ,  $R = H$ ) with  $Pb(OAc)_4$  in  $CH_2Cl_2$  results in the intramol. addition of the N-nitrene to the triple bond in each case and azirines II ( $m = 1$ ,  $R = H$ , Me;  $m = 2$ ,  $R = H$ ) are isolated. An x-ray crystal structure determination of II ( $m = 1$ ,  $R = H$ ) reveals a remarkable deformation of bond angles at the spiro center and this feature appears to be common to all azirines. The five membered ring in II ( $m = 1$ ) has the envelope conformation and the six-membered ring in II ( $m = 2$ ) has the twist-boat conformation; a possible explanation for this conformational anchoring is offered.

RX(7) OF 260 ...P ==> Q...

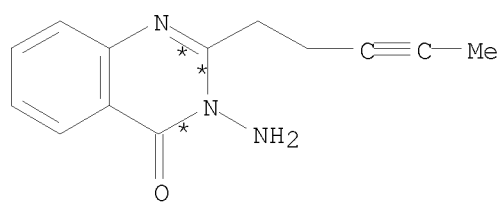


10/ 562,112



P

(7)  $\longrightarrow$

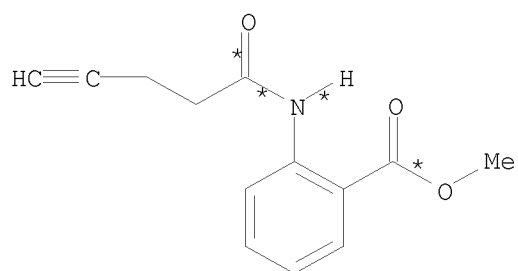


Q

YIELD 90%

RX(7)	RCT	P	107428-13-7
	RGT	R	302-01-2 N2H4
	PRO	Q	98750-79-9
	SOL		64-17-5 EtOH

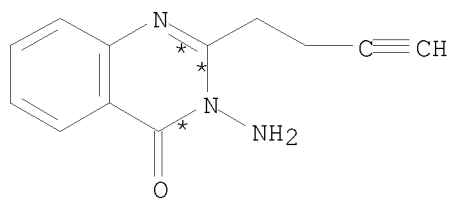
RX(8) OF 260      ...S ==> T...



S

(8)  $\longrightarrow$

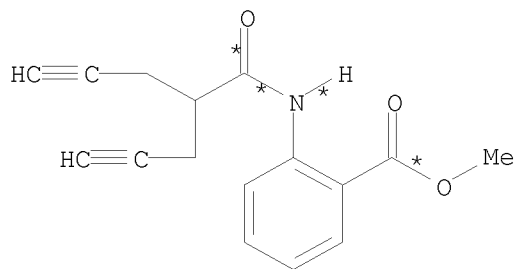
10/ 562,112



T  
YIELD 46%

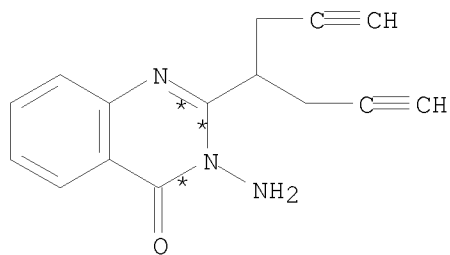
RX(8)        RCT    S 107428-12-6  
              RGT    R 302-01-2 N2H4  
              PRO    T 98750-77-7  
              SOL    64-17-5 EtOH

RX(14) OF 260        ...AD ==> AA...



AD

(14)

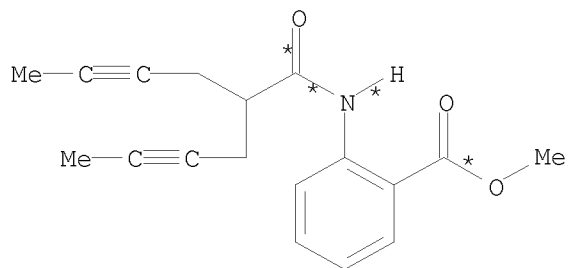


AA  
YIELD 63%

RX(14)        RCT    AD 107428-15-9  
              RGT    R 302-01-2 N2H4  
              PRO    AA 98750-78-8  
              SOL    64-17-5 EtOH  
              NTE    Product varies with reactors tiime

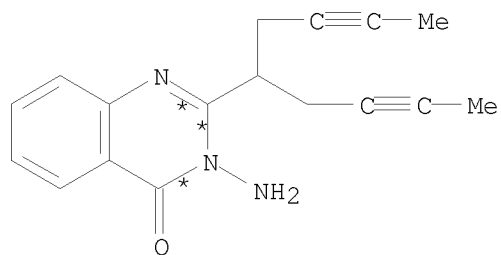
10/ 562,112

RX(16) OF 260 ...AF ==> AG...



AF

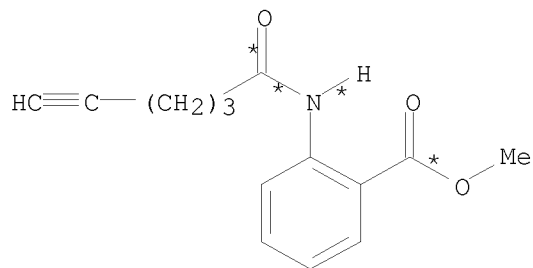
(16)



AG  
YIELD 59%

RX(16)     RCT   AF 107428-16-0  
           RGT   R 302-01-2 N2H4  
           PRO   AG 107428-08-0  
           SOL   64-17-5 EtOH

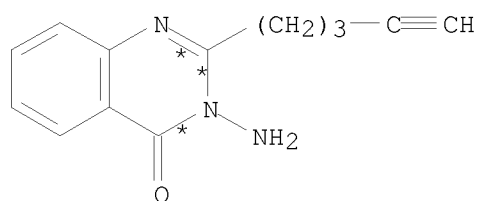
RX(18) OF 260 ...AI ==> AJ...



AI

(18)

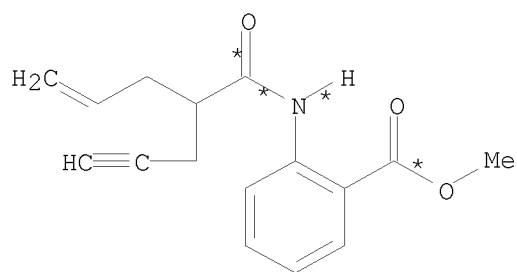
10/ 562,112



AJ  
YIELD 70%

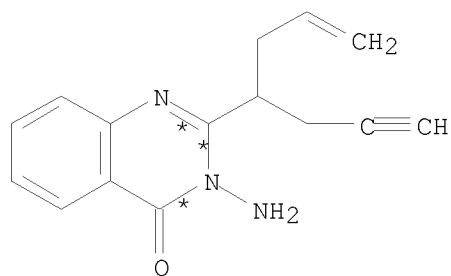
RX(18)      RCT    AI 107428-14-8  
              RGT    R 302-01-2 N<sub>2</sub>H<sub>4</sub>  
              PRO    AJ 98750-87-9  
              SOL    64-17-5 EtOH

RX(39) OF 260      ...BJ ==> BK...



BJ

(39) ➤



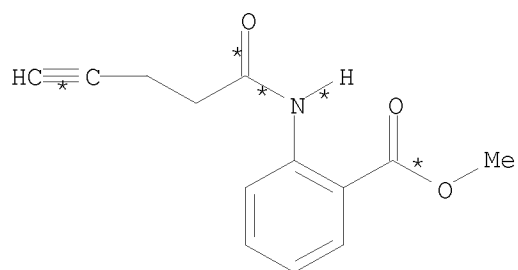
BK

RX(39)      RCT    BJ 107428-21-7  
              RGT    R 302-01-2 N<sub>2</sub>H<sub>4</sub>  
              PRO    BK 107428-22-8  
              SOL    64-17-5 EtOH

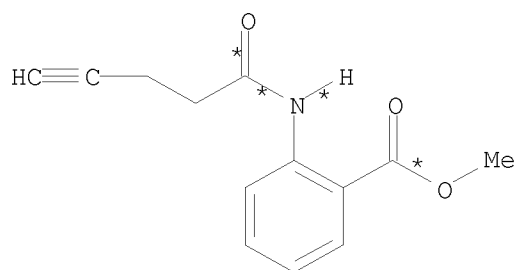
RX(55) OF 260 COMPOSED OF RX(8), RX(10)

10/ 562,112

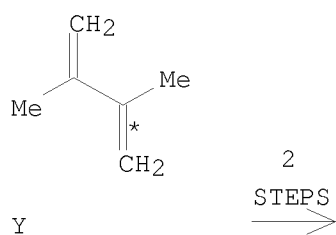
RX(55)      2 S + Y ==> V + Z



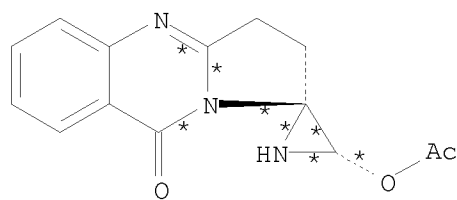
S



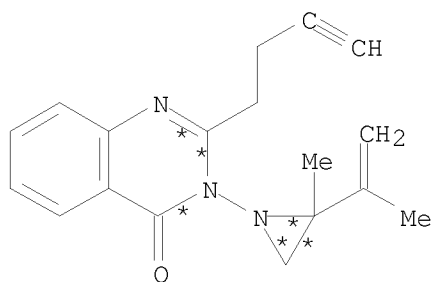
S



Y



V



Z

RX(8)      RCT   S 107428-12-6  
              RGT   R 302-01-2 N2H4  
              PRO   T 98750-77-7  
              SOL   64-17-5 EtOH

RX(10)      RCT   T 98750-77-7

STAGE(1)

RGT   W 546-67-8 Pb(OAc)4  
 SOL   75-09-2 CH2Cl2

STAGE(2)

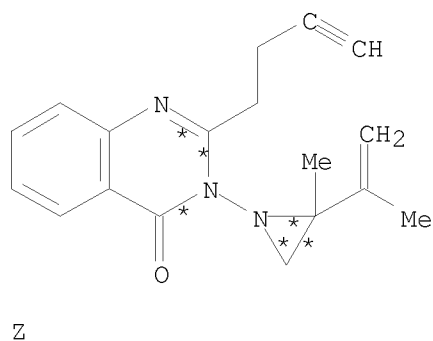
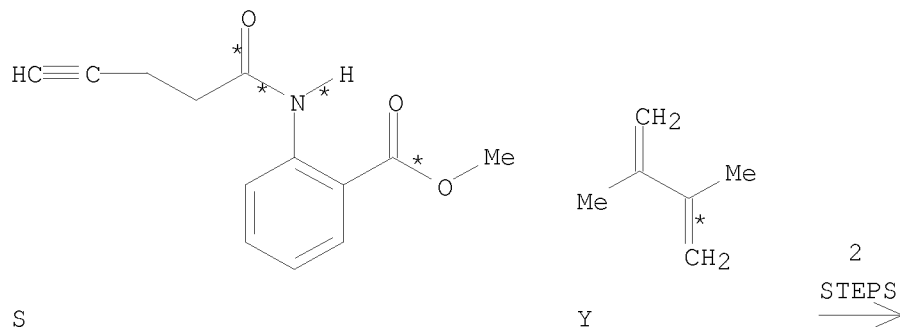
RCT   Y 513-81-5

PRO   V 98750-85-7, Z 107428-11-5

10/ 562,112

RX(56) OF 260 COMPOSED OF RX(8), RX(11)

RX(56) S + Y ==> Z



RX(8) RCT S 107428-12-6  
RGT R 302-01-2 N2H4  
PRO T 98750-77-7  
SOL 64-17-5 EtOH

RX(11) RCT Y 513-81-5, T 98750-77-7  
RGT W 546-67-8 Pb(OAc)4  
PRO Z 107428-11-5  
SOL 75-09-2 CH2Cl2

L3 ANSWER 187 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 106:102196 CASREACT

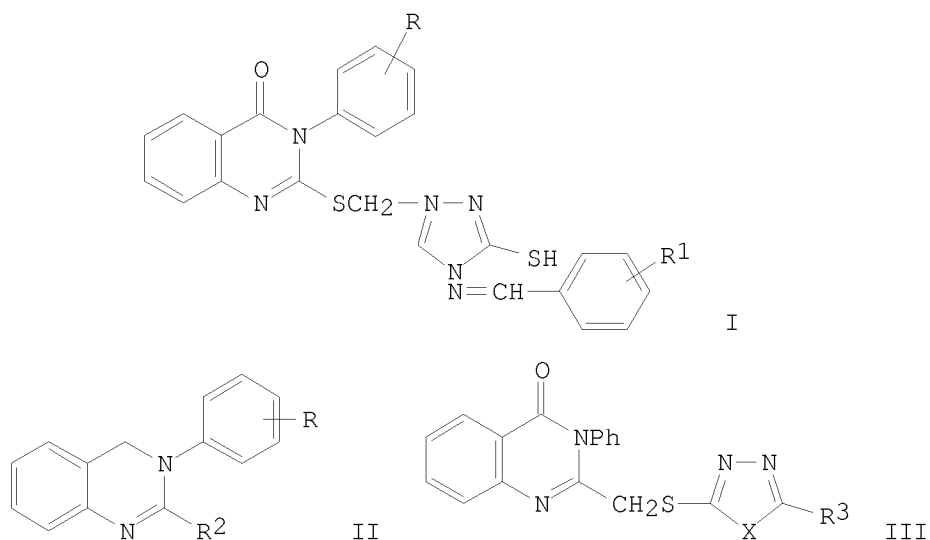
TITLE: Synthesis of certain new sulfur-containing  
quinazolinone derivatives likely to possess CNS  
depressant action

AUTHOR(S): El-Feky, S. A.; Al-Ashmawi, M. I.; Hazzaa, A. A. B.;  
El-Fattah, B. Abd

CORPORATE SOURCE: Fac. Pharm., Zagazig Univ., Egypt

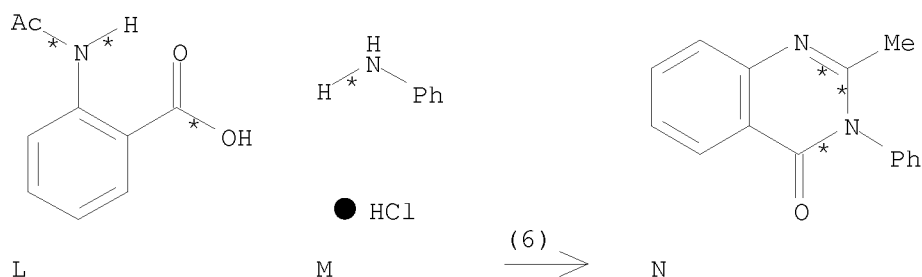
SOURCE: Egyptian Journal of Pharmaceutical Sciences (1985),  
Volume Date 1983, 24(1-4), 39-47  
CODEN: EJPSBZ; ISSN: 0301-5068

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Quinazolines I ( $R = H, 2\text{-Me}, 4\text{-Me}$ ;  $R_1 = H, 4\text{-Cl}, 3\text{-NO}_2, 4\text{-NO}_2, 4\text{-MeO}, 2\text{-OH}, 4\text{-OH}$ ) were prepared from amides II ( $R_2 = \text{SCH}_2\text{CONHNH}_2$ ), by dithiocarboxylation followed by cyclocondensation with  $\text{N}_2\text{H}_4$  and condensation of  $\text{R}_1\text{C}_6\text{H}_4\text{CHO}$ . Condensation of II ( $R_1 = H, R_2 = \text{CH}_2\text{Br}$ ) with triazoles and oxadiazoles yielded compds. III ( $X = O, \text{NNH}_2$ ; by dithiocarboxylation followed by cyclocondensation with  $\text{N}_2\text{H}_4$  and condensation with  $\text{R}_1\text{C}_6\text{H}_4\text{CHO}$ . Condensation of II ( $R_1 = H, R_2 = \text{CH}_2\text{Br}$ ) with triazoles and oxadiazoles yielded compds. III ( $X = O, \text{NNH}_2$ ;  $R_3 = \text{Ph}, 3\text{-pyridyl}, 4\text{-pyridyl}, 4\text{-ClC}_6\text{H}_4\text{OCH}_2, Z = \text{ClC}_6\text{H}_4\text{OCH}_2$ ). The anticonvulsant activity of several I-III were tested (no data).

RX(6) OF 169 ...L + M ==> N...

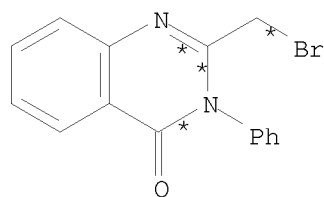
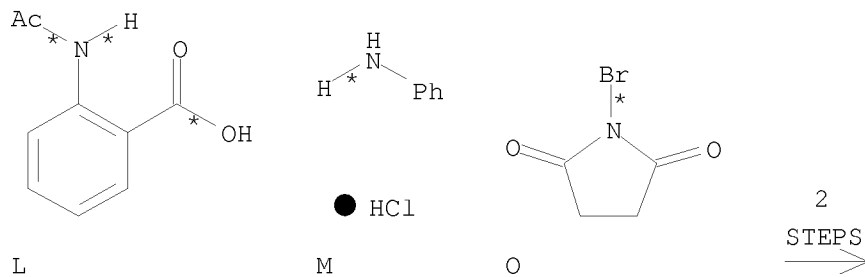


RX(6) RCT L 89-52-1, M 142-04-1  
 PRO N 2385-23-1

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RX(46) OF 169 COMPOSED OF RX(6), RX(7)

RX(46) L + M + O ==> P



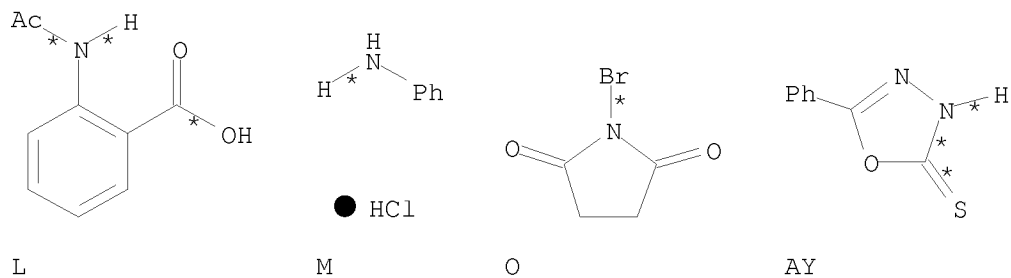
P

RX(6) RCT L 89-52-1, M 142-04-1  
PRO N 2385-23-1

RX(7) RCT N 2385-23-1, O 128-08-5  
PRO P 19062-58-9

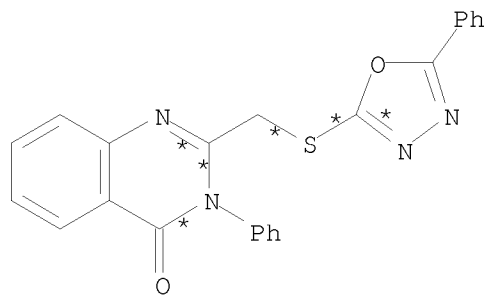
RX(85) OF 169 COMPOSED OF RX(6), RX(7), RX(32)

RX(85) L + M + O + AY ==> AZ





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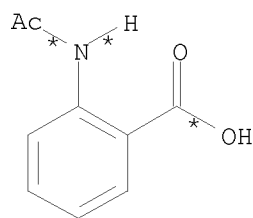
AZ

RX(6) RCT L 89-52-1, M 142-04-1  
PRO N 2385-23-1

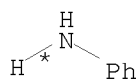
RX(7) RCT N 2385-23-1, O 128-08-5  
PRO P 19062-58-9

RX(32) RCT P 19062-58-9, AY 3004-42-0  
PRO AZ 105491-93-8  
SOL 67-64-1 Me2CO

RX(86) OF 169 COMPOSED OF RX(6), RX(7), RX(33)  
RX(86) L + M + O + BB ==> BC

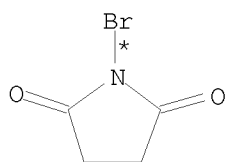


L

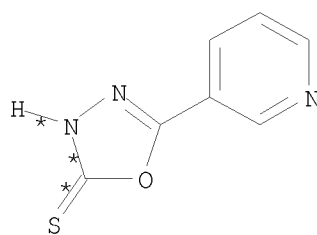


M

● HCl



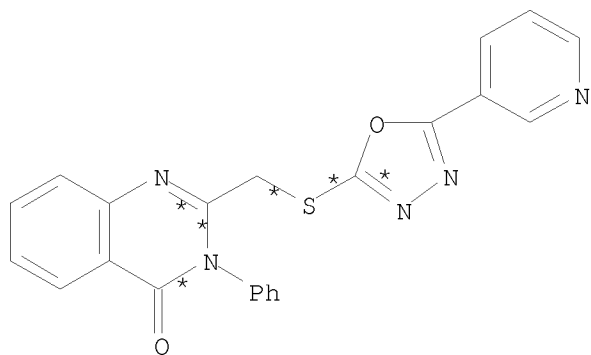
O



BB

3  
STEPS  
→

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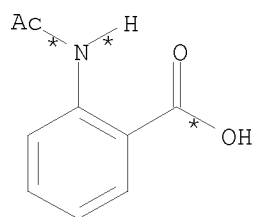
BC

RX(6) RCT L 89-52-1, M 142-04-1  
PRO N 2385-23-1

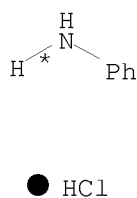
RX(7) RCT N 2385-23-1, O 128-08-5  
PRO P 19062-58-9

RX(33) RCT P 19062-58-9, BB 3690-46-8  
PRO BC 105491-94-9  
SOL 67-64-1 Me2CO

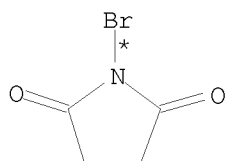
RX(87) OF 169 COMPOSED OF RX(6), RX(7), RX(34)  
RX(87) L + M + O + BD ==> BE



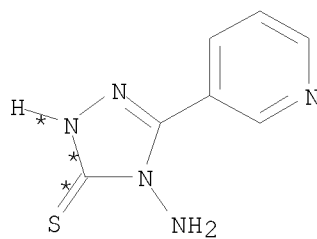
L



M

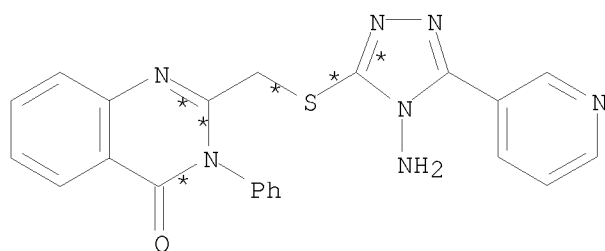


O



BD

3  
STEPS  
→



BE

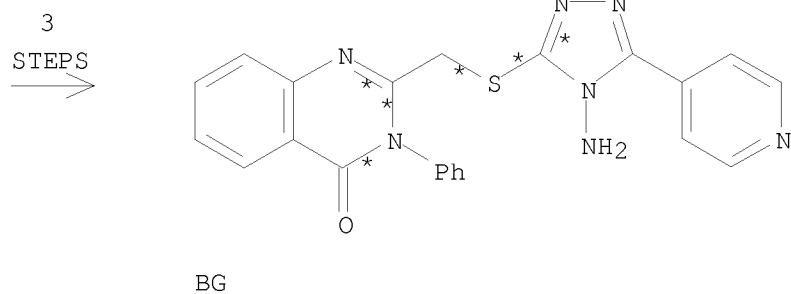
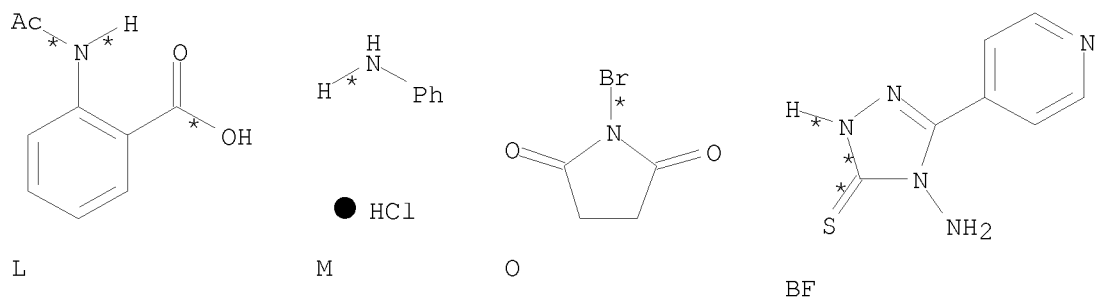
10/ 562,112

RX(6) RCT L 89-52-1, M 142-04-1  
PRO N 2385-23-1

RX(7) RCT N 2385-23-1, O 128-08-5  
PRO P 19062-58-9

RX(34) RCT P 19062-58-9, BD 78027-00-6  
PRO BE 105491-97-2  
SOL 67-64-1 Me2CO

RX(88) OF 169 COMPOSED OF RX(6), RX(7), RX(35)  
RX(88) L + M + O + BF ==> BG



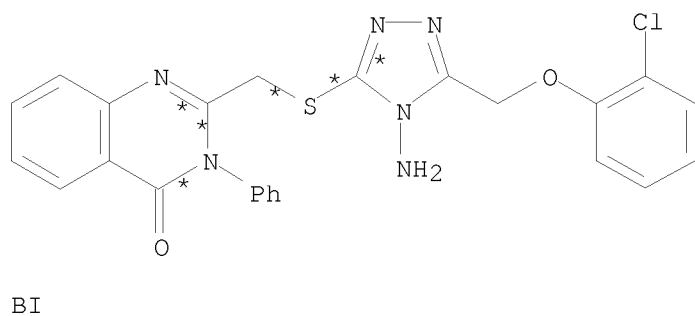
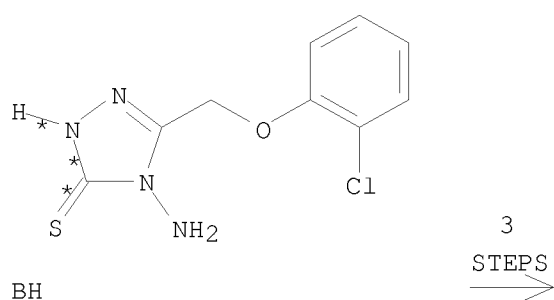
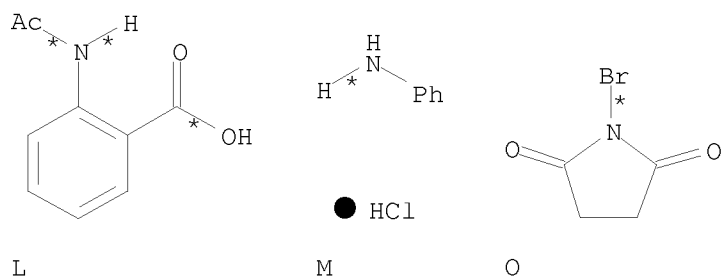
RX(6) RCT L 89-52-1, M 142-04-1  
PRO N 2385-23-1

RX(7) RCT N 2385-23-1, O 128-08-5  
PRO P 19062-58-9

RX(35) RCT P 19062-58-9, BF 36209-51-5  
PRO BG 105491-98-3  
SOL 67-64-1 Me2CO

RX(89) OF 169 COMPOSED OF RX(6), RX(7), RX(36)  
RX(89) L + M + O + BH ==> BI

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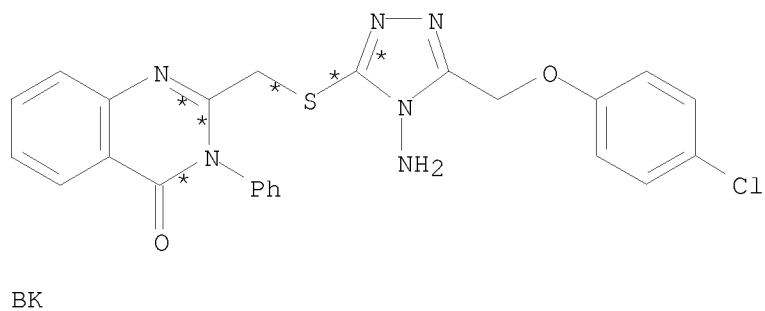
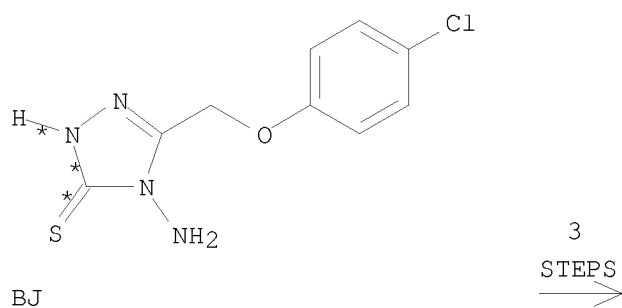
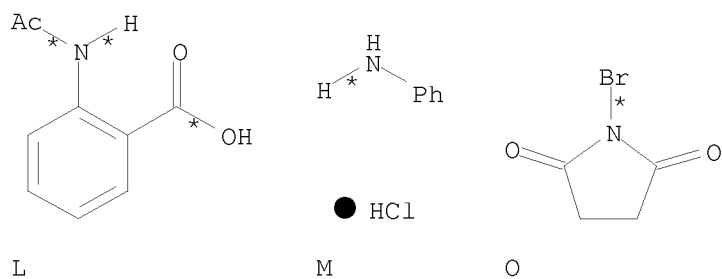
RX(6)      RCT    L 89-52-1, M 142-04-1  
              PRO    N 2385-23-1

RX(7)      RCT    N 2385-23-1, O 128-08-5  
              PRO    P 19062-58-9

RX(36)     RCT    P 19062-58-9, BH 4413-42-7  
              PRO    BI 105491-99-4  
              SOL    67-64-1 Me2CO

RX(90) OF 169 COMPOSED OF RX(6), RX(7), RX(37)  
 RX(90)      L + M + O + BJ ==> BK

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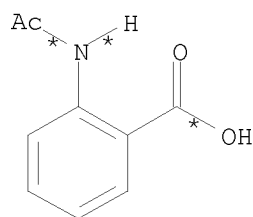
RX(6)      RCT    L 89-52-1, M 142-04-1  
             PRO    N 2385-23-1

RX(7)      RCT    N 2385-23-1, O 128-08-5  
             PRO    P 19062-58-9

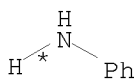
RX(37)     RCT    P 19062-58-9, BJ 4413-43-8  
             PRO    BK 105492-00-0  
             SOL    67-64-1 Me2CO

RX(91) OF 169 COMPOSED OF RX(6), RX(7), RX(40)  
 RX(91)      L + M + O + BM ==> BN

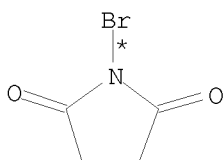
10/ 562,112



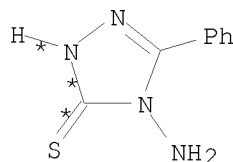
L



M

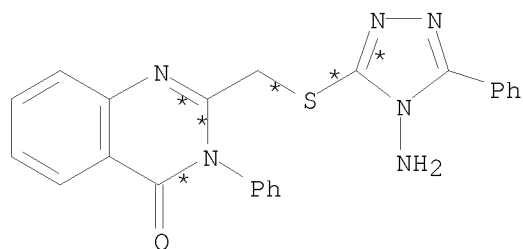


O



BM

3  
STEPS  
→



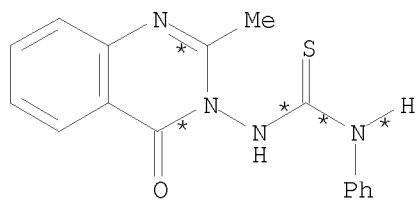
BN

RX(6)	RCT	L 89-52-1, M 142-04-1
	PRO	N 2385-23-1
RX(7)	RCT	N 2385-23-1, O 128-08-5
	PRO	P 19062-58-9
RX(40)	RCT	P 19062-58-9, BM 22706-11-2
	PRO	BN 105491-96-1
	SOL	67-64-1 Me2CO

L3 ANSWER 188 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 106:50150 CASREACT  
TITLE: Possible antiParkinsonian compounds. Synthesis of  
2-styryl-3-arylthiouryl-3,4-dihydro-4-oxoquinazolines  
Pandey, V. K.  
AUTHOR(S):  
CORPORATE SOURCE: Dep. Chem., Univ. Lucknow, Lucknow, 226 001, India  
SOURCE: Current Science (1986), 55(5), 243-6  
CODEN: CUSCAM; ISSN: 0011-3891  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



10/ 562,112

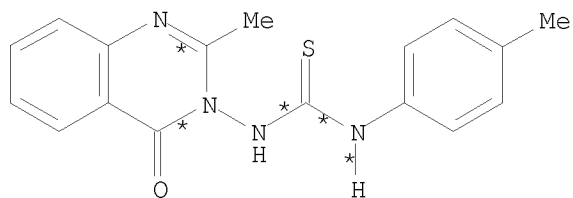
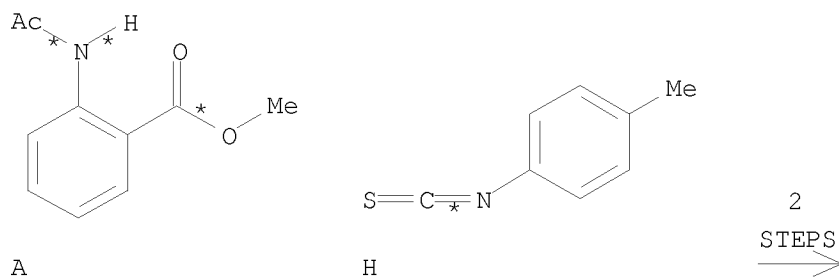


G  
YIELD 50%

RX(1) RCT A 2719-08-6  
RGT C 302-01-2 N2H4  
PRO B 1898-06-2

RX(3) RCT B 1898-06-2, F 103-72-0  
PRO G 62495-71-0

RX(13) OF 36 COMPOSED OF RX(1), RX(4)  
RX(13) A + H ==> I



I  
YIELD 50%

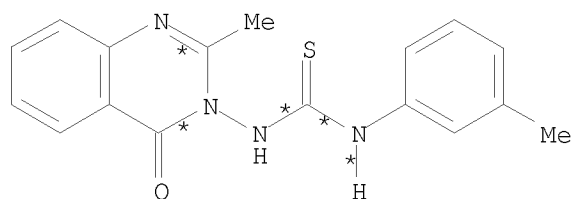
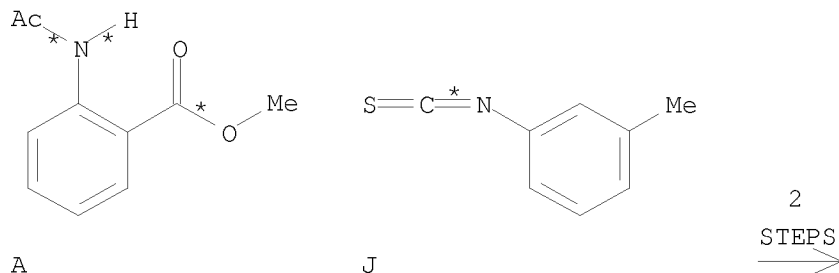
RX(1) RCT A 2719-08-6  
RGT C 302-01-2 N2H4  
PRO B 1898-06-2

RX(4) RCT B 1898-06-2, H 622-59-3  
PRO I 87200-42-8



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RX(14) OF 36 COMPOSED OF RX(1), RX(5)  
RX(14)     A   +   J   ==>   K

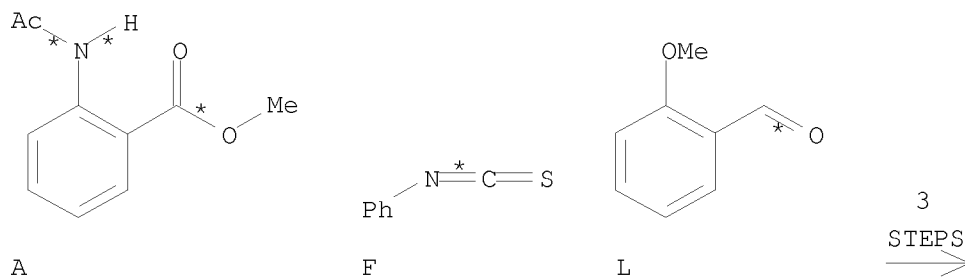


K  
YIELD 50%

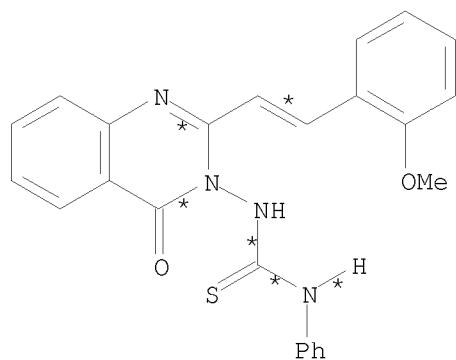
RX(1)     RCT   A 2719-08-6  
           RGT   C 302-01-2 N2H4  
           PRO   B 1898-06-2

RX(5)     RCT   B 1898-06-2, J 621-30-7  
           PRO   K 105886-56-4

RX(22) OF 36 COMPOSED OF RX(1), RX(3), RX(6)  
RX(22)     A   +   F   +   L   ==>   M



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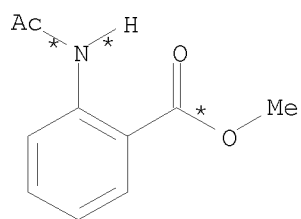
M  
YIELD 30%

RX(1)      RCT    A 2719-08-6  
             RGT    C 302-01-2 N2H4  
             PRO    B 1898-06-2

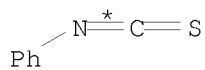
RX(3)      RCT    B 1898-06-2, F 103-72-0  
             PRO    G 62495-71-0

RX(6)      RCT    G 62495-71-0, L 135-02-4  
             PRO    M 105886-57-5

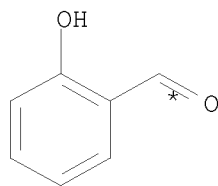
RX(23) OF 36 COMPOSED OF RX(1), RX(3), RX(7)  
RX(23)      A + F + N ==> O



A



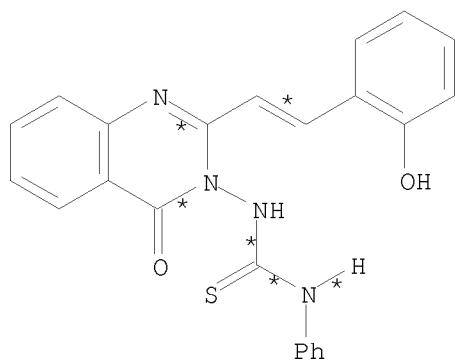
F



N

3  
STEPS  
→

10/ 562,112



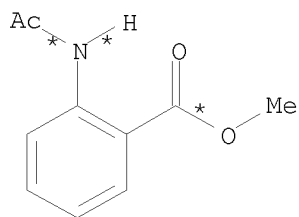
O  
YIELD 30%

RX(1) RCT A 2719-08-6  
RGT C 302-01-2 N2H4  
PRO B 1898-06-2

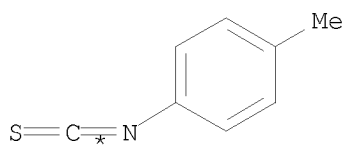
RX(3) RCT B 1898-06-2, F 103-72-0  
PRO G 62495-71-0

RX(7) RCT G 62495-71-0, N 90-02-8  
PRO O 105886-58-6

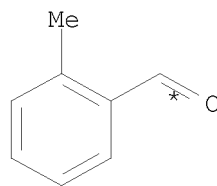
RX(24) OF 36 COMPOSED OF RX(1), RX(4), RX(8)  
RX(24) A + H + P ==> Q



A



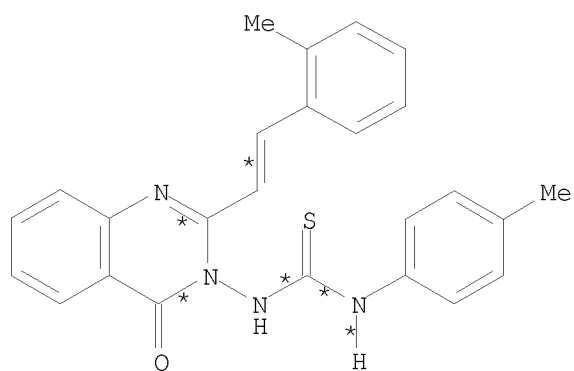
H



P

3  
STEPS  
→

10/ 562,112



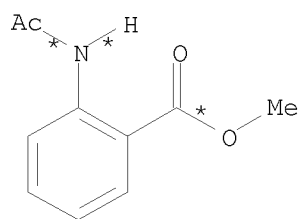
Q  
YIELD 90%

RX(1) RCT A 2719-08-6  
RGT C 302-01-2 N2H4  
PRO B 1898-06-2

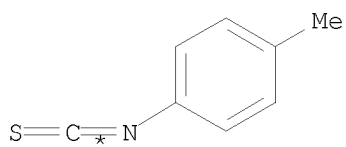
RX(4) RCT B 1898-06-2, H 622-59-3  
PRO I 87200-42-8

RX(8) RCT I 87200-42-8, P 529-20-4  
PRO Q 105886-59-7

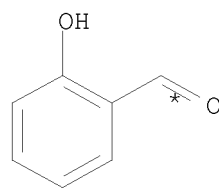
RX(25) OF 36 COMPOSED OF RX(1), RX(4), RX(9)  
RX(25) A + H + N ==> R



A



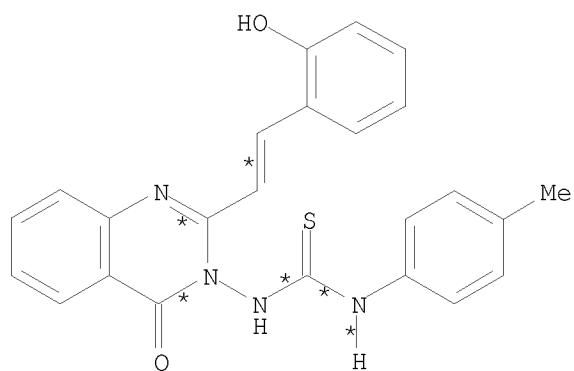
H



N

3  
STEPS  
→

10/ 562,112



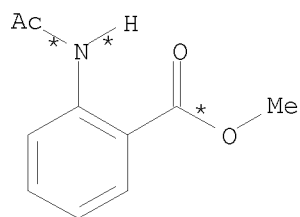
R  
YIELD 30%

RX(1) RCT A 2719-08-6  
RGT C 302-01-2 N2H4  
PRO B 1898-06-2

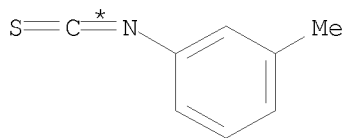
RX(4) RCT B 1898-06-2, H 622-59-3  
PRO I 87200-42-8

RX(9) RCT I 87200-42-8, N 90-02-8  
PRO R 105886-60-0

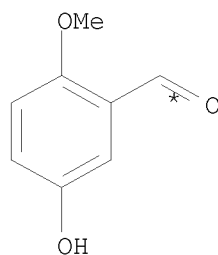
RX(26) OF 36 COMPOSED OF RX(1), RX(5), RX(10)  
RX(26) A + J + S ==> T



A



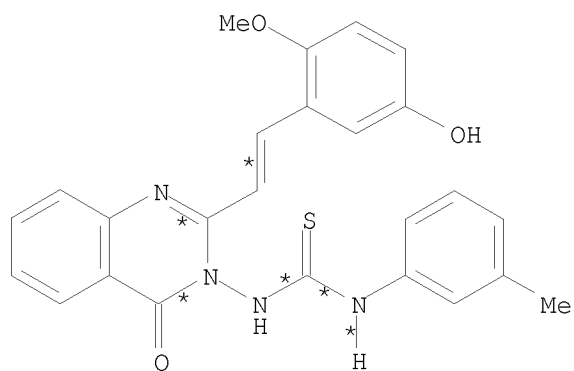
J



S

3  
STEPS  
→

10/ 562,112



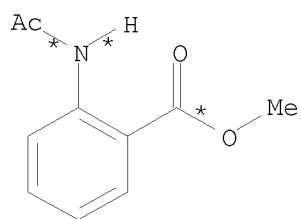
T  
YIELD 30%

RX(1) RCT A 2719-08-6  
RGT C 302-01-2 N2H4  
PRO B 1898-06-2

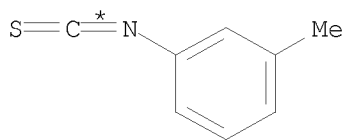
RX(5) RCT B 1898-06-2, J 621-30-7  
PRO K 105886-56-4

RX(10) RCT K 105886-56-4, S 35431-26-6  
PRO T 105886-61-1

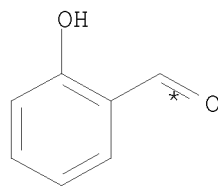
RX(27) OF 36 COMPOSED OF RX(1), RX(5), RX(11)  
RX(27) A + J + N ==> U



A



J

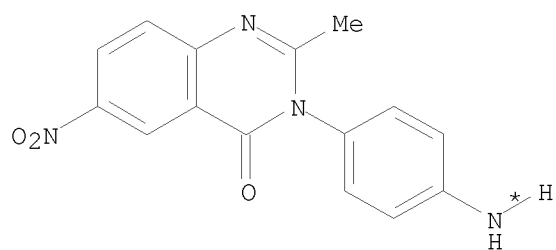


N

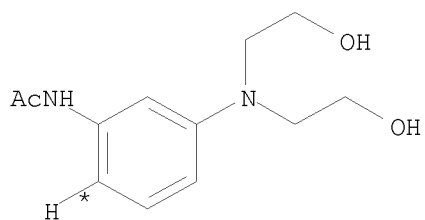
3  
STEPS  
→



10/ 562,112

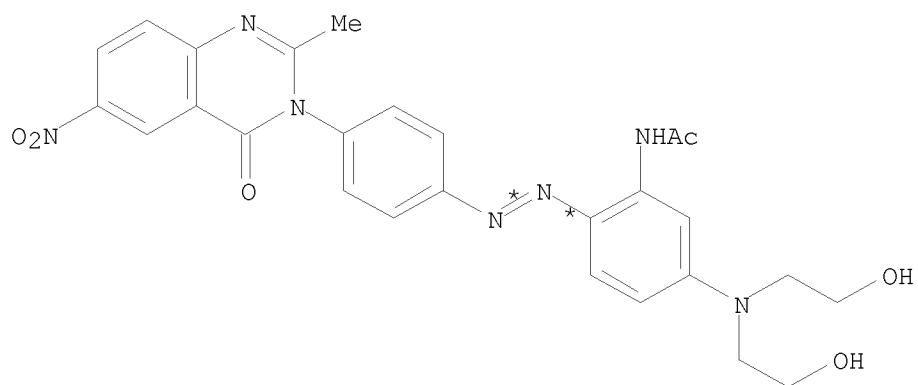


A



AS

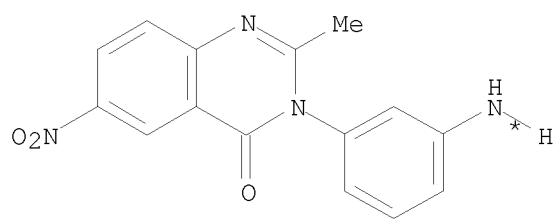
(29)  $\longrightarrow$



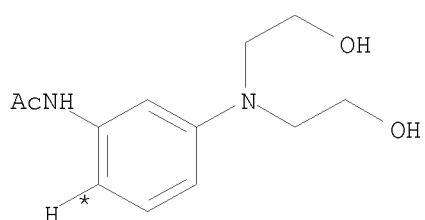
AT

RX(29) RCT A 105440-62-8, AS 92-02-4  
PRO AT 105440-79-7

RX(30) OF 30 D + AS ==> AU



D

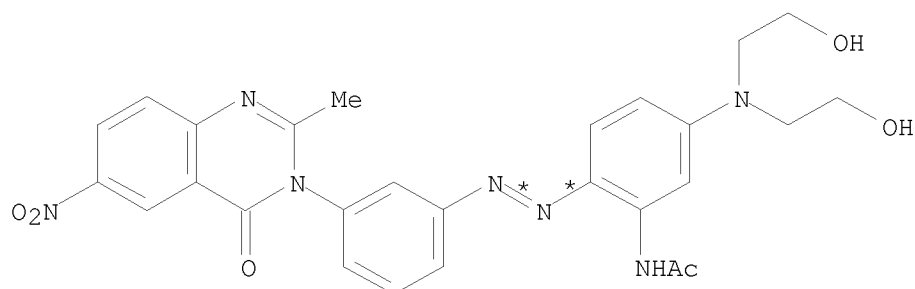


AS



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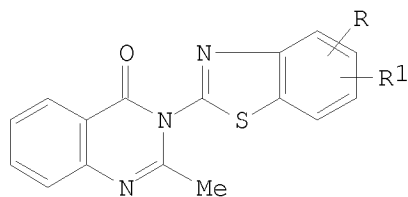
(30)  
→



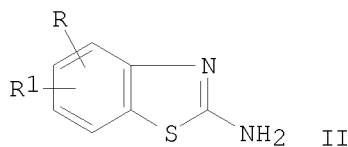
AU

RX(30) RCT D 105440-63-9, AS 92-02-4  
PRO AU 105440-95-7

L3 ANSWER 190 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 105:226481 CASREACT  
TITLE: Synthesis of some new  
3-(2'-benzothiazolyl)-4(3H)-quinazolinones as  
antifungal agents  
AUTHOR(S): Lakhan, Ram; Rai, Babban J.  
CORPORATE SOURCE: Dep. Chem., Banaras Hindu Univ., Varanasi, 221 005,  
India  
SOURCE: Journal of Chemical and Engineering Data (1986),  
31(4), 501-2  
CODEN: JCEAAX; ISSN: 0021-9568  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



I

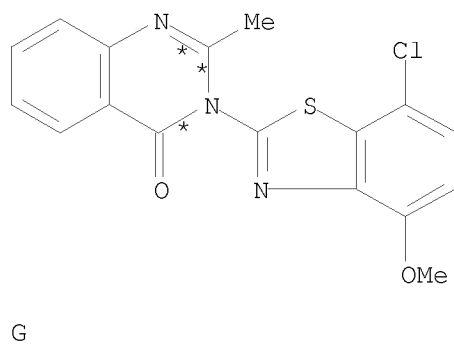
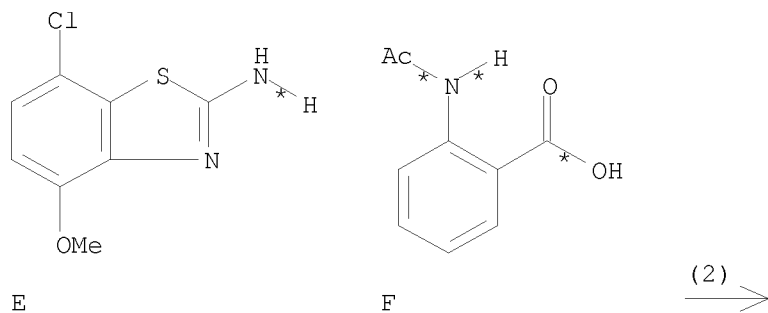


II

AB The title compds. I (R = 5-, 6-NO<sub>2</sub>, R<sub>1</sub> = H; R = 4-MeO, R<sub>1</sub> = 7-Cl; R = 4-NO<sub>2</sub>, R<sub>1</sub> = 6-Cl, R = 4-Cl, R<sub>1</sub> = 6-NO<sub>2</sub>) were prepared in 66-72% yield by the cyclization of o-MeCONHC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H with aminobenzothiazoles II. I (R = 5-, 6-NO<sub>2</sub>, R<sub>1</sub> = H; R = 4-Cl, R<sub>1</sub> = 6-NO<sub>2</sub>) had fungicidal activity comparable with that of Dithan M-45.

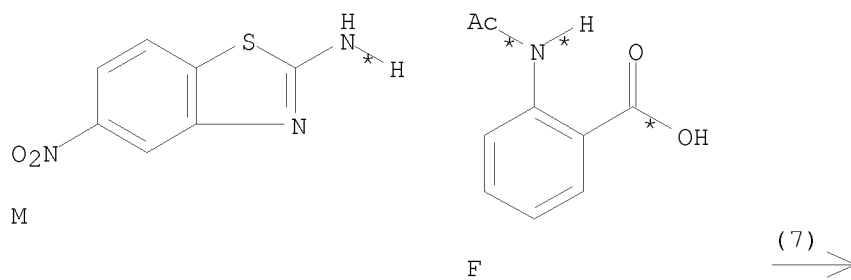
10/ 562,112

RX(2) OF 15      ...E + F ==> G

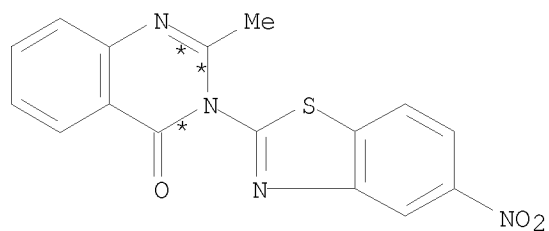


RX(2)      RCT   E 67618-12-6, F 89-52-1  
RGT   H 7719-12-2 PC13  
PRO   G 103852-54-6  
SOL   108-88-3 PhMe

RX(7) OF 15      ...M + F ==> Q



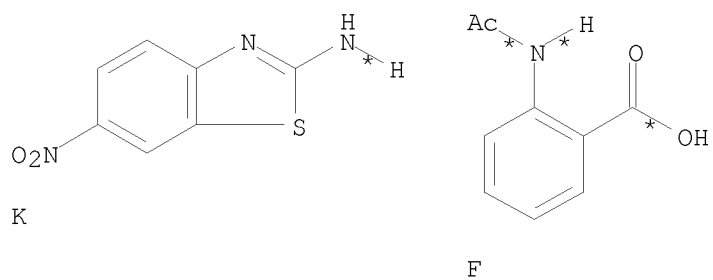
10/ 562,112



Q

RX(7) RCT M 73458-39-6, F 89-52-1  
RGT H 7719-12-2 PC13  
PRO Q 103852-52-4  
SOL 108-88-3 PhMe

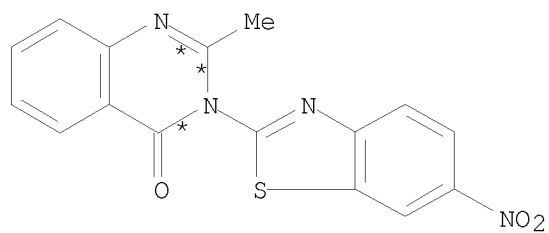
RX(8) OF 15 ...K + F ==> R



K

F

(8) →

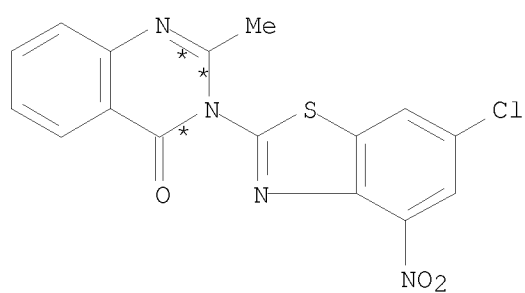
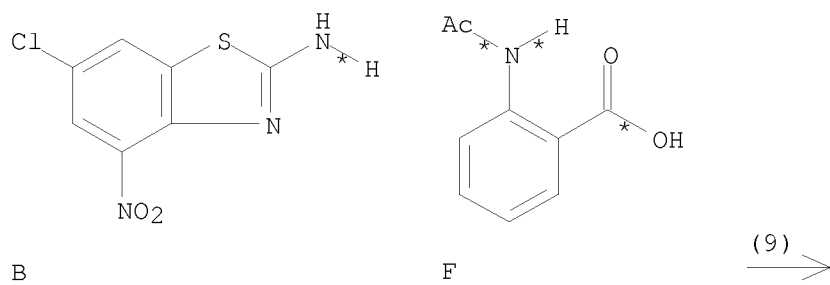


R

RX(8) RCT K 6285-57-0, F 89-52-1  
RGT H 7719-12-2 PC13  
PRO R 103852-53-5  
SOL 108-88-3 PhMe

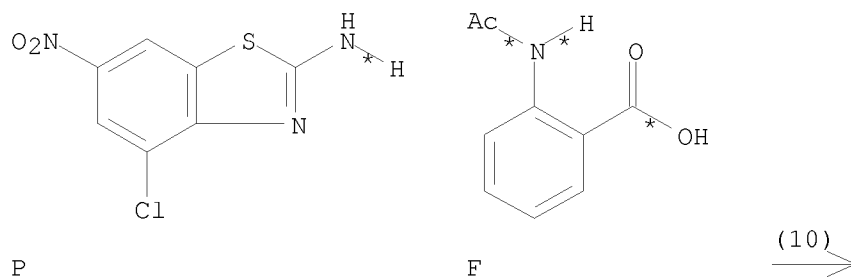
RX(9) OF 15 ...B + F ==> S

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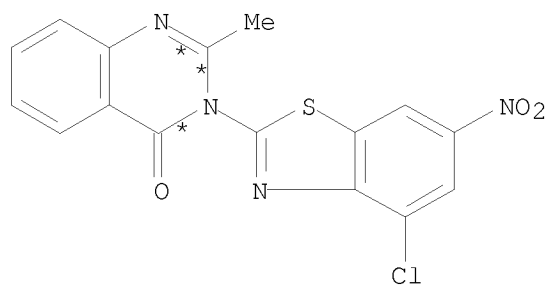


RX(9) RCT B 26488-55-1, F 89-52-1  
RGT H 7719-12-2 PC13  
PRO S 103852-55-7  
SOL 108-88-3 PhMe

RX(10) OF 15 ...P + F ==> T



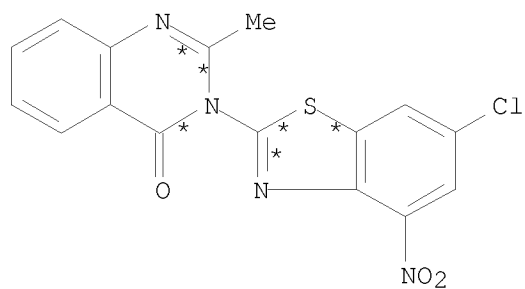
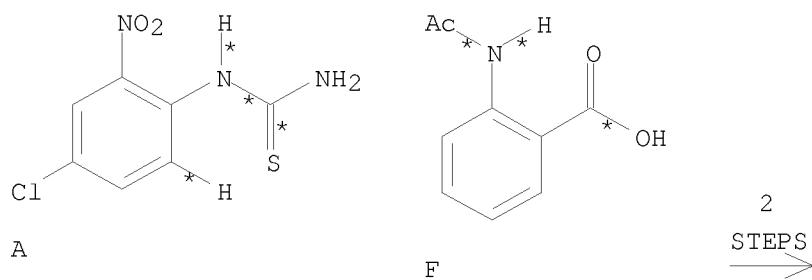
10/ 562,112



T

RX(10)      RCT   P 66188-30-5, F 89-52-1  
               RGT   H 7719-12-2 PC13  
               PRO   T 103852-56-8  
               SOL   108-88-3 PhMe

RX(11) OF 15 COMPOSED OF RX(1), RX(9)  
 RX(11)      A   +   F   ==>   S



S

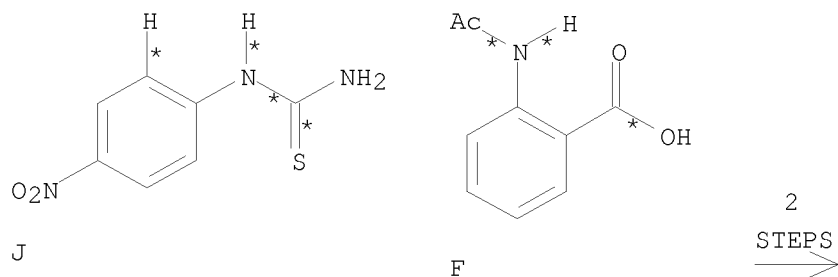
RX(1)      RCT   A 39535-50-7  
               RGT   C 7726-95-6 Br2  
               PRO   B 26488-55-1  
               SOL   67-66-3 CHCl3

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RX(9)        RCT   B 26488-55-1, F 89-52-1  
              RGT   H 7719-12-2 PC13  
              PRO   S 103852-55-7  
              SOL   108-88-3 PhMe

RX(12) OF 15 COMPOSED OF RX(3), RX(8)

RX(12)       J   +   F   ==>   R



R

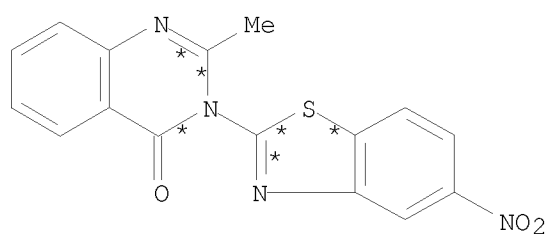
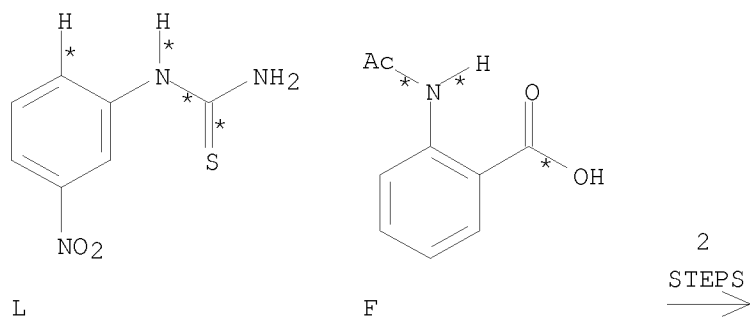
RX(3)        RCT   J 3696-22-8  
              RGT   C 7726-95-6 Br2  
              PRO   K 6285-57-0  
              SOL   67-66-3 CHCl3

RX(8)        RCT   K 6285-57-0, F 89-52-1  
              RGT   H 7719-12-2 PC13  
              PRO   R 103852-53-5  
              SOL   108-88-3 PhMe

RX(13) OF 15 COMPOSED OF RX(4), RX(7)

RX(13)       L   +   F   ==>   Q

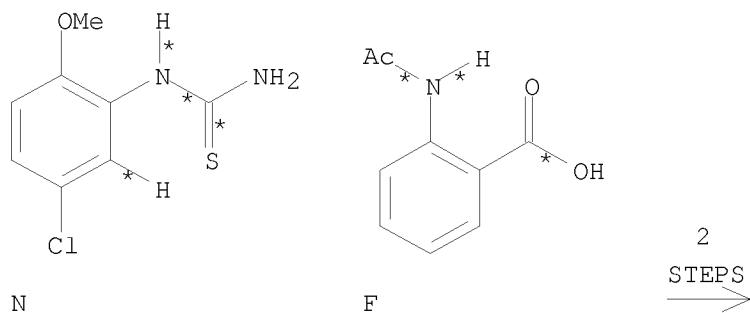
10/ 562,112



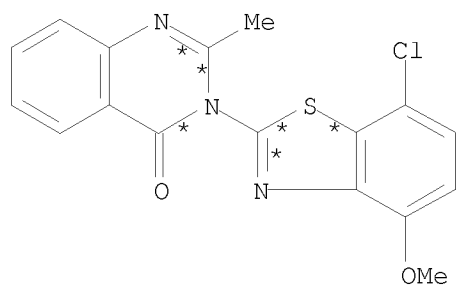
Q

RX(4)	RCT	L 709-72-8
	RGT	C 7726-95-6 Br2
	PRO	M 73458-39-6
	SOL	67-66-3 CHCl3
RX(7)	RCT	M 73458-39-6, F 89-52-1
	RGT	H 7719-12-2 PCl3
	PRO	Q 103852-52-4
	SOL	108-88-3 PhMe

RX(14) OF 15 COMPOSED OF RX(5), RX(2)  
 RX(14) N + F ==> G



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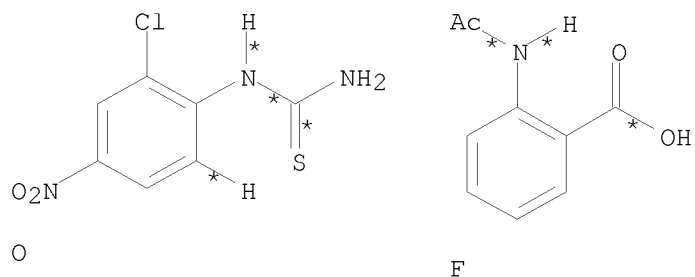
G

RX(5) RCT N 63980-69-8  
 RGT C 7726-95-6 Br2  
 PRO E 67618-12-6  
 SOL 67-66-3 CHCl3

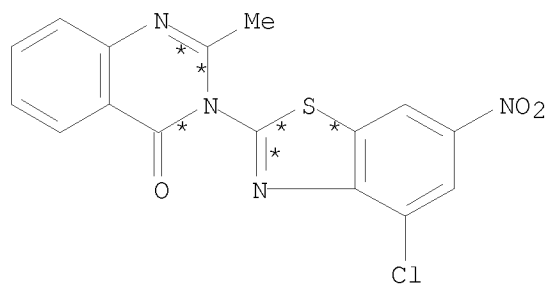
RX(2) RCT E 67618-12-6, F 89-52-1  
 RGT H 7719-12-2 PC13  
 PRO G 103852-54-6  
 SOL 108-88-3 PhMe

RX(15) OF 15 COMPOSED OF RX(6), RX(10)

RX(15) O + F ==> T



2  
 STEPS  
 →



T

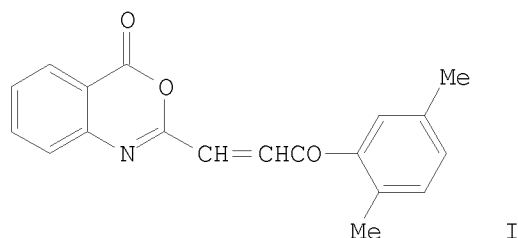


10/ 562,112

RX(6) RCT O 103852-57-9  
RGT C 7726-95-6 Br2  
PRO P 66188-30-5  
SOL 67-66-3 CHCl3

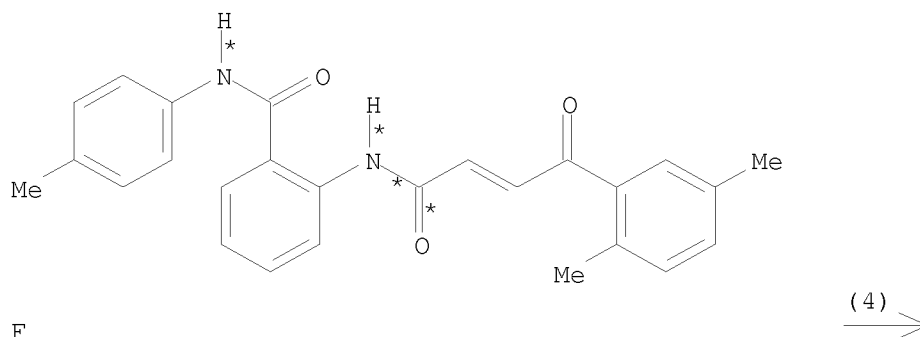
RX(10) RCT P 66188-30-5, F 89-52-1  
RGT H 7719-12-2 PC13  
PRO T 103852-56-8  
SOL 108-88-3 PhMe

L3 ANSWER 191 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 105:226465 CASREACT  
TITLE: Synthesis and some reactions of new  
3,1-benzoxazin-4-one derivatives  
AUTHOR(S): Soliman, E. A.; Attia, I. A.; Guber, A. M.  
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt  
SOURCE: Egyptian Journal of Chemistry (1985), 27(3), 297-308  
CODEN: EGJCA3; ISSN: 0367-0422  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

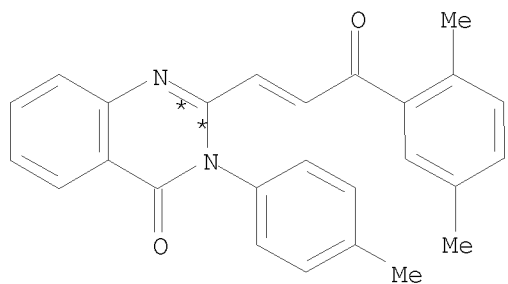


AB Benzoxazinone I was prepared by treating 2-HO2CC6H4NH2 with 2,5-Me2C6H3COCH:CHCOCl and cyclization of 2-HO2CC6H4NHCOCH:CHCOC6H3Me2-2,5 with Ac2O. I reacted with amines, hydrazines, NH2OH, ureas, and thioureas to form various heterocyclic derivs.

RX(4) OF 37 ...F ==> J



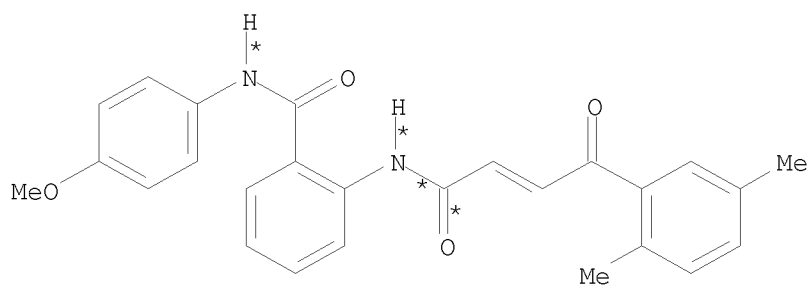
10/ 562,112



J

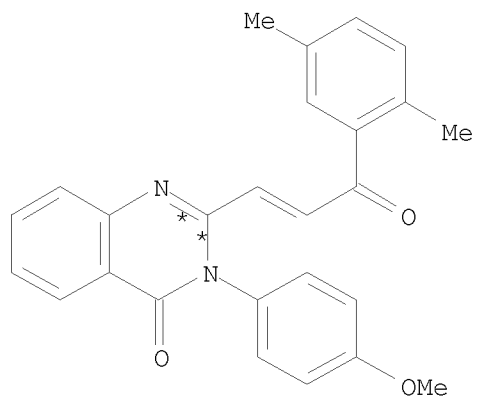
RX(4) RCT F 105493-09-2  
PRO J 105493-11-6  
CAT 108-24-7 Ac2O

RX(6) OF 37 ...I ==> M



I

(6)  $\longrightarrow$

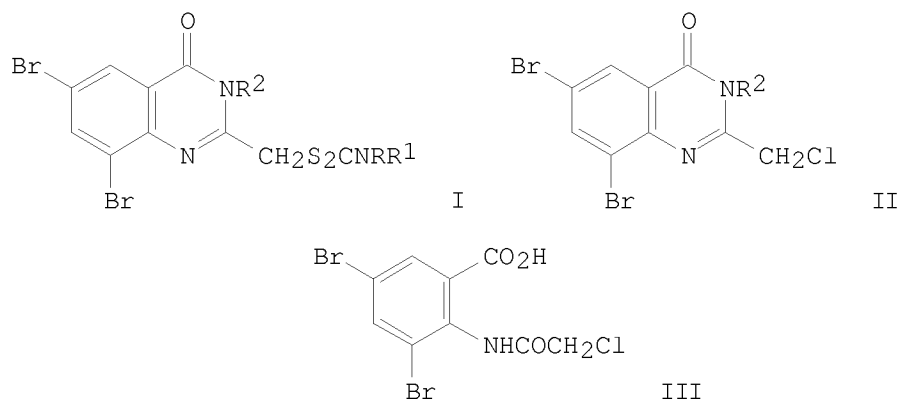


M

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RX(6) RCT I 105493-10-5  
PRO M 105493-12-7  
CAT 108-24-7 Ac2O

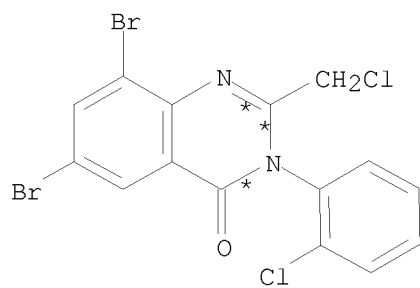
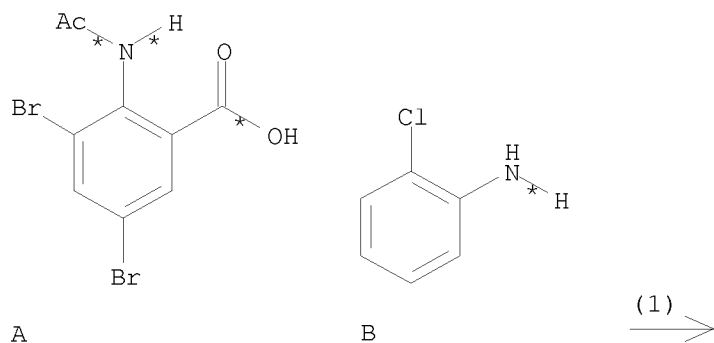
L3 ANSWER 192 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 105:133835 CASREACT  
TITLE: Synthesis and biological activities of  
[6,8-dibromo-3-aryl-3,4-dihydro-4-oxo-2-  
quinazolinyl]methyl N-substituted dithiocarbamates  
AUTHOR(S): Rao, A. Devender; Shankar, C. Ravi; Reddy, V. Malla  
CORPORATE SOURCE: Coll. Pharm. Sci., Kakatiya Univ., Warangal, 506 009,  
India  
SOURCE: Current Science (1985), 54(15), 720-2  
CODEN: CUSCAM; ISSN: 0011-3891  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Quinzaolinylmethyl dithiocarbamates I [R = H, cyclohexyl; R1 = Ph, C6H4Me-4, C6H4OEt-4, C6H4OMe-4, PhCH2, cyclohexyl, Me2N(CH2)3; RR1 = (CH2)4, (CH2)5, (CH2)20(CH2)2, (CH2)2NPh(CH2)2] were prepared by condensation of (chloromethyl)quinazoline II (R2 = C6H4Cl-2, CH2C6H4OMe-2) with RR1NCS2H. A mixture of anthranilic acid III, 2-chloroaniline, and POC13 in PhMe was refluxed at 130-140° for 3 h to give 72% II (R2 = C6H4Cl-2). I showed fungicidal and insecticidal activity.

RX(1) OF 40 A + B ==> C...

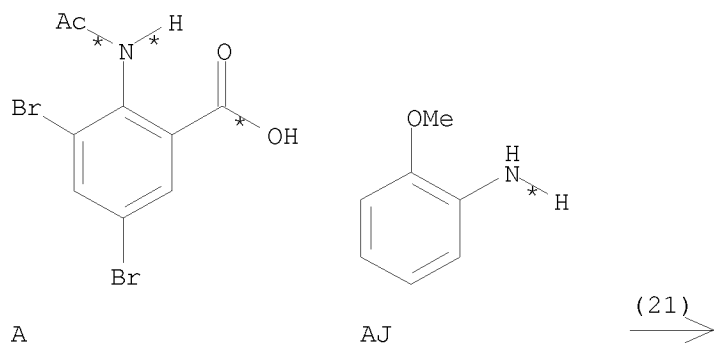
10/ 562,112



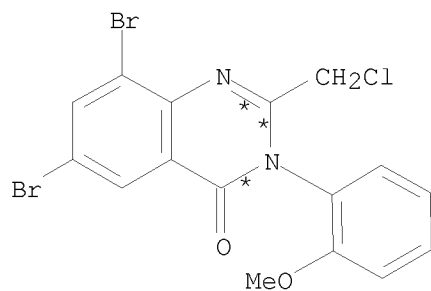
C  
YIELD 72%

RX(1)      RCT    A 16610-45-0, B 95-51-2  
              RGT    D 10025-87-3 POC13  
              PRO    C 104308-98-7

RX(21) OF 40      A + AJ ==> AA...



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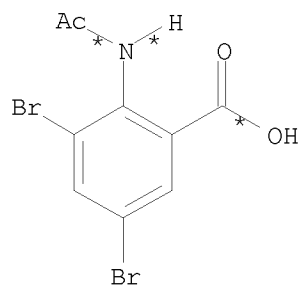


AA

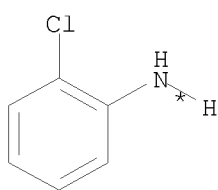
RX(21) RCT A 16610-45-0, AJ 90-04-0  
RGT D 10025-87-3 POC13  
PRO AA 104308-99-8

RX(22) OF 40 COMPOSED OF RX(1), RX(2)

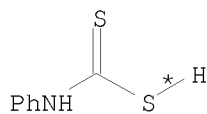
RX(22) A + B + E ==> F



A

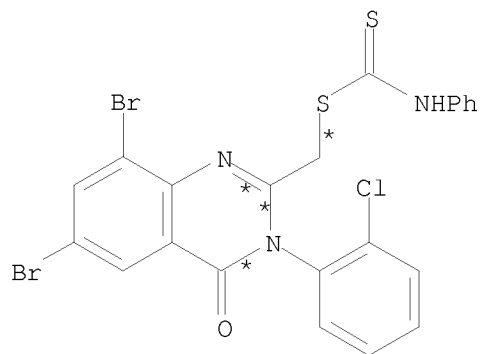


B



E

2  
STEPS  
→



F

RX(1) RCT A 16610-45-0, B 95-51-2

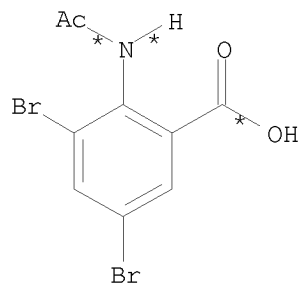
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RGT D 10025-87-3 POC13  
PRO C 104308-98-7

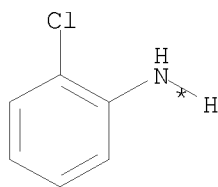
RX(2) RCT C 104308-98-7, E 1074-52-8  
PRO F 104329-30-8

RX(23) OF 40 COMPOSED OF RX(1), RX(3)

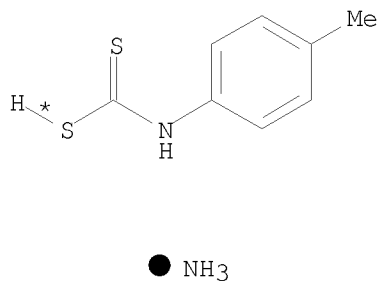
RX(23) A + B + G ==> H



A

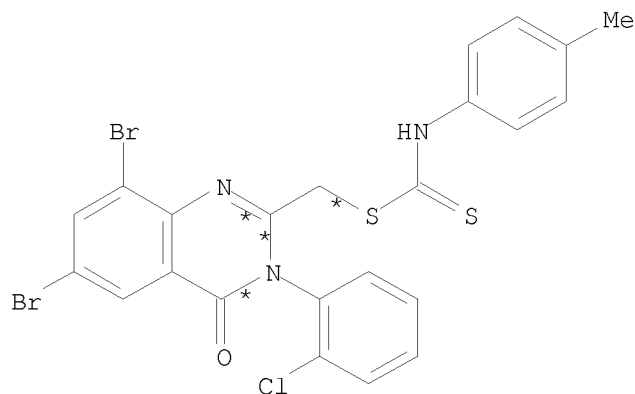


B



G

2  
STEPS  
=>



H

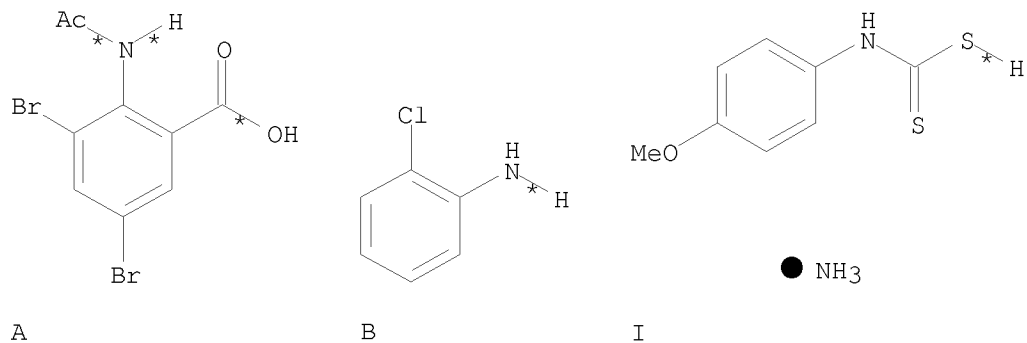
RX(1) RCT A 16610-45-0, B 95-51-2  
RGT D 10025-87-3 POC13  
PRO C 104308-98-7

RX(3) RCT C 104308-98-7, G 13036-91-4  
PRO H 104308-78-3

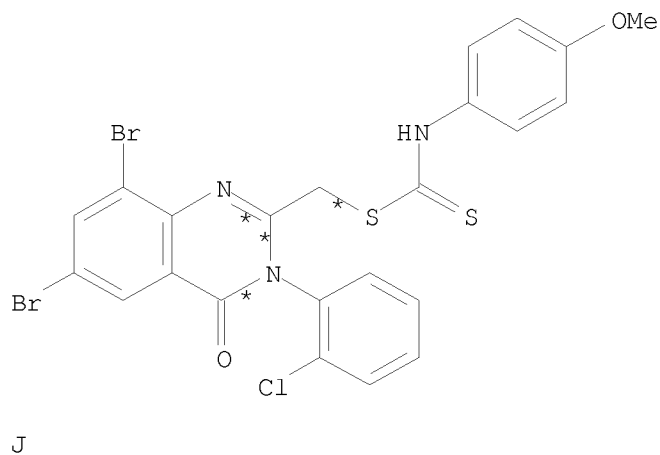
RX(24) OF 40 COMPOSED OF RX(1), RX(4)

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RX(24)      A + B + I ==> J



2  
STEPS  
→

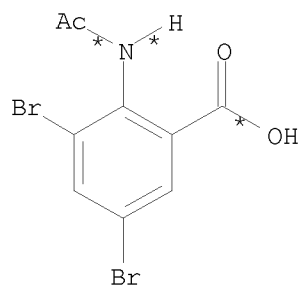


RX(1)      RCT    A 16610-45-0, B 95-51-2  
             RGT    D 10025-87-3 POC13  
             PRO    C 104308-98-7

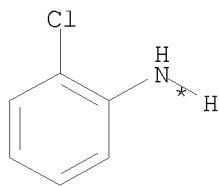
RX(4)      RCT    C 104308-98-7, I 15866-98-5  
             PRO    J 104308-79-4

RX(25) OF 40 COMPOSED OF RX(1), RX(5)  
RX(25)      A + B + K ==> L

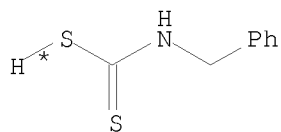
10/ 562,112



A



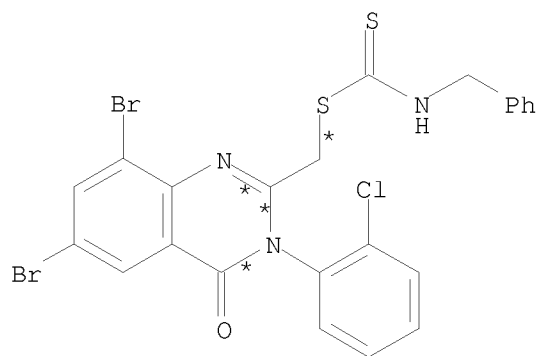
B



K



2  
STEPS  
→



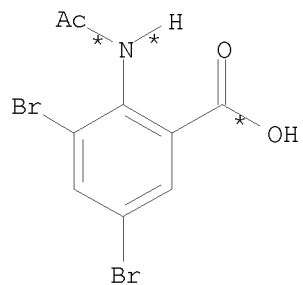
L

RX(1) RCT A 16610-45-0, B 95-51-2  
RGT D 10025-87-3 POC13  
PRO C 104308-98-7

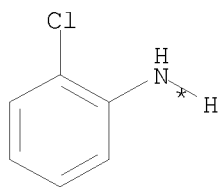
RX(5) RCT C 104308-98-7, K 41270-27-3  
PRO L 104308-80-7

RX(26) OF 40 COMPOSED OF RX(1), RX(6)

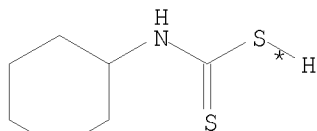
RX(26) A + B + M ==> N



A



B



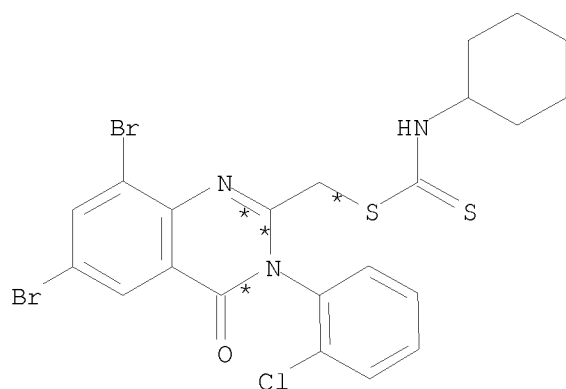
M





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2  
STEPS  
→

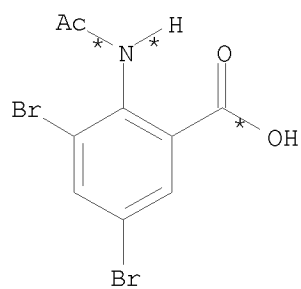


N

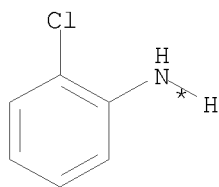
RX(1) RCT A 16610-45-0, B 95-51-2  
RGT D 10025-87-3 POC13  
PRO C 104308-98-7

RX(6) RCT C 104308-98-7, M 66917-87-1  
PRO N 104329-32-0

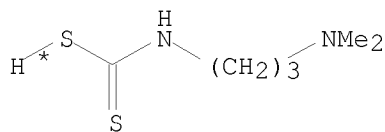
RX(27) OF 40 COMPOSED OF RX(1), RX(7)  
RX(27) A + B + O ==> P



A



B

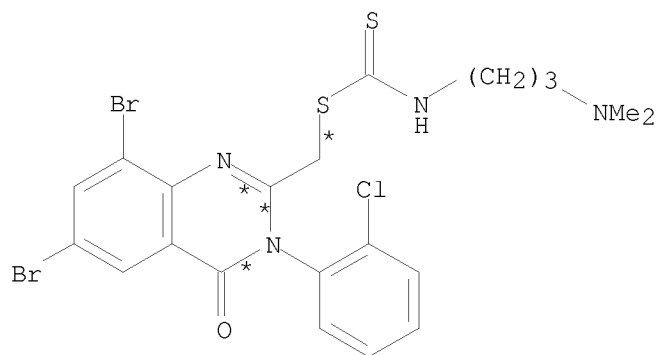


O



2  
STEPS  
→

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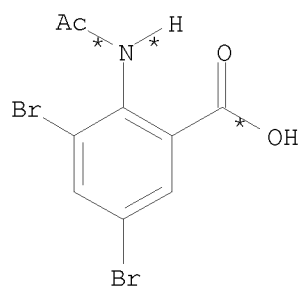


P

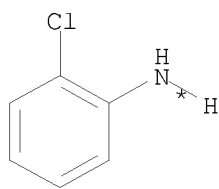
RX(1) RCT A 16610-45-0, B 95-51-2  
 RGT D 10025-87-3 POC13  
 PRO C 104308-98-7

RX(7) RCT C 104308-98-7, O 200131-07-3  
 PRO P 104308-81-8

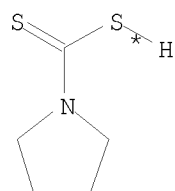
RX(28) OF 40 COMPOSED OF RX(1), RX(8)  
 RX(28) A + B + Q ==> R



A



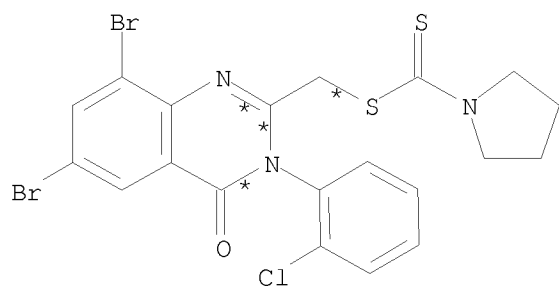
B



● NH3  
 Q

2  
 STEPS  
 →

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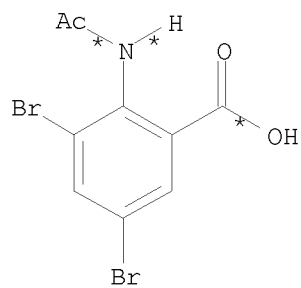


R  
YIELD 72%

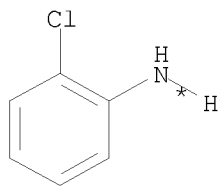
RX(1) RCT A 16610-45-0, B 95-51-2  
RGT D 10025-87-3 POC13  
PRO C 104308-98-7

RX(8) RCT C 104308-98-7, Q 5108-96-3  
PRO R 104329-33-1

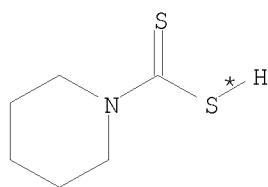
RX(29) OF 40 COMPOSED OF RX(1), RX(9)  
RX(29) A + B + S ==> T



A



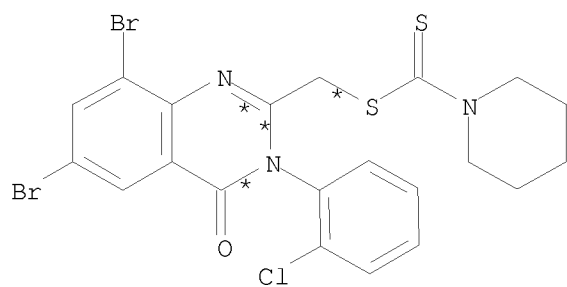
B



S

● NH<sub>3</sub>

2  
STEPS  
→



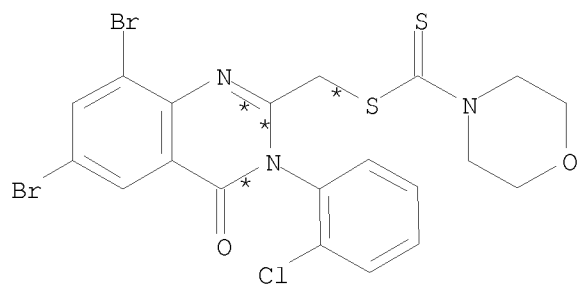
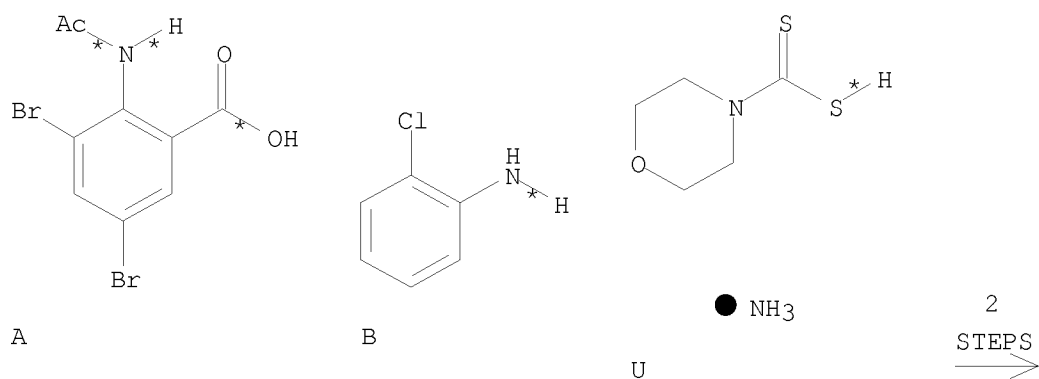
T

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RX(1) RCT A 16610-45-0, B 95-51-2  
RGT D 10025-87-3 POC13  
PRO C 104308-98-7

RX(9) RCT C 104308-98-7, S 49791-55-1  
PRO T 104308-82-9

RX(30) OF 40 COMPOSED OF RX(1), RX(10)  
RX(30) A + B + U ==> V



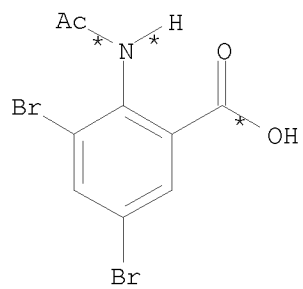
V

RX(1) RCT A 16610-45-0, B 95-51-2  
RGT D 10025-87-3 POC13  
PRO C 104308-98-7

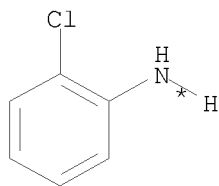
RX(10) RCT C 104308-98-7, U 49791-54-0  
PRO V 104308-83-0

RX(31) OF 40 COMPOSED OF RX(1), RX(11)  
RX(31) A + B + W ==> X

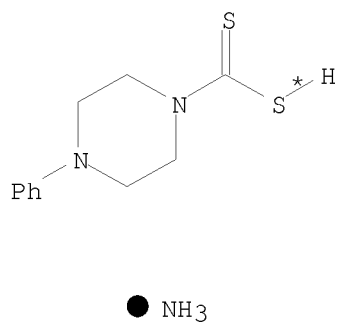
10/ 562,112



A

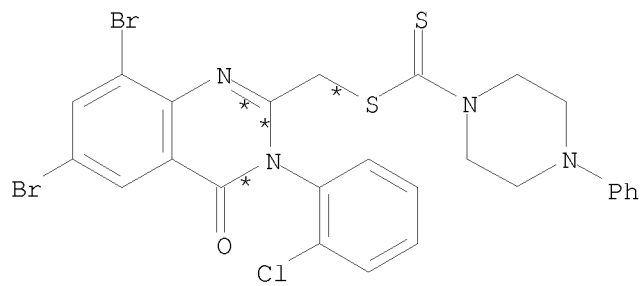


B



W

2  
STEPS  
→



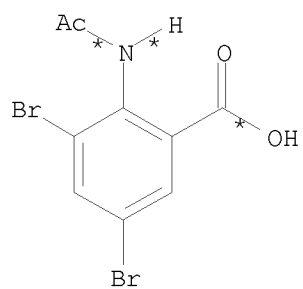
X

RX(1) RCT A 16610-45-0, B 95-51-2  
RGT D 10025-87-3 POC13  
PRO C 104308-98-7

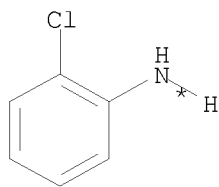
RX(11) RCT C 104308-98-7, W 100805-68-3  
PRO X 104308-84-1

RX(32) OF 40 COMPOSED OF RX(1), RX(12)  
RX(32) A + B + Y ==> Z

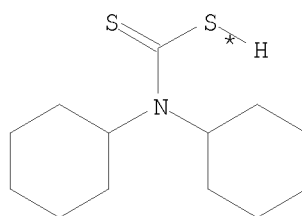
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A



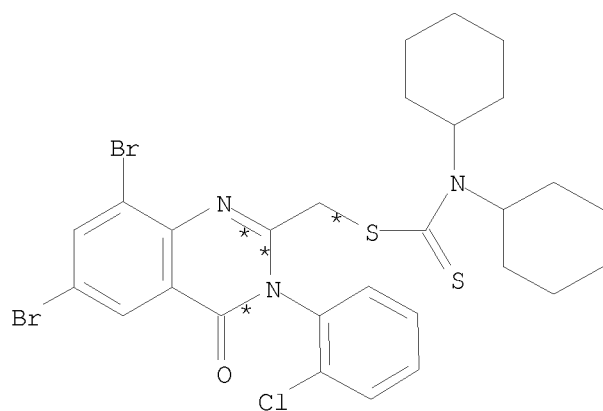
B



● NH<sub>3</sub>

Y

2  
STEPS  
→



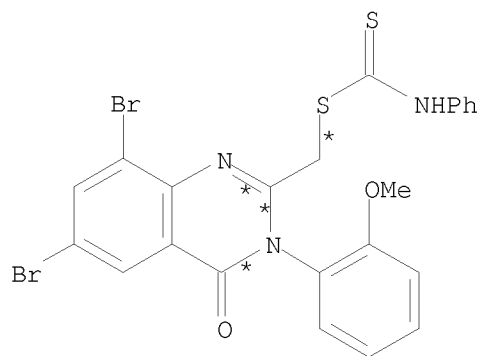
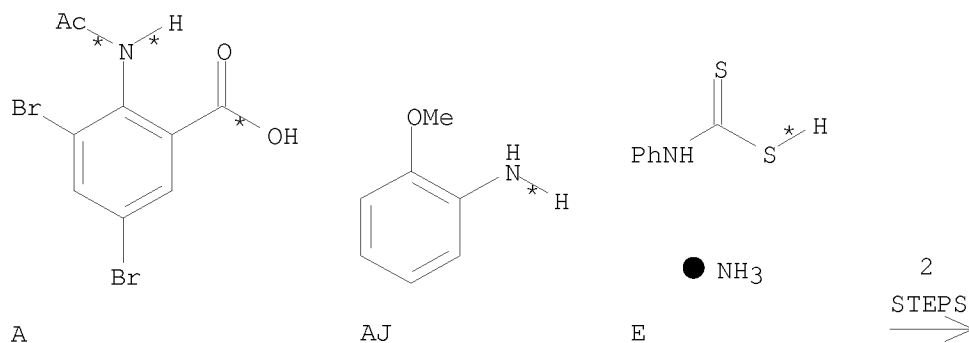
Z

RX(1)      RCT    A 16610-45-0, B 95-51-2  
             RGT    D 10025-87-3 POC13  
             PRO    C 104308-98-7

RX(12)     RCT    C 104308-98-7, Y 100805-67-2  
             PRO    Z 104308-85-2

RX(33) OF 40 COMPOSED OF RX(21), RX(13)  
RX(33)      A + AJ + E ==> AB

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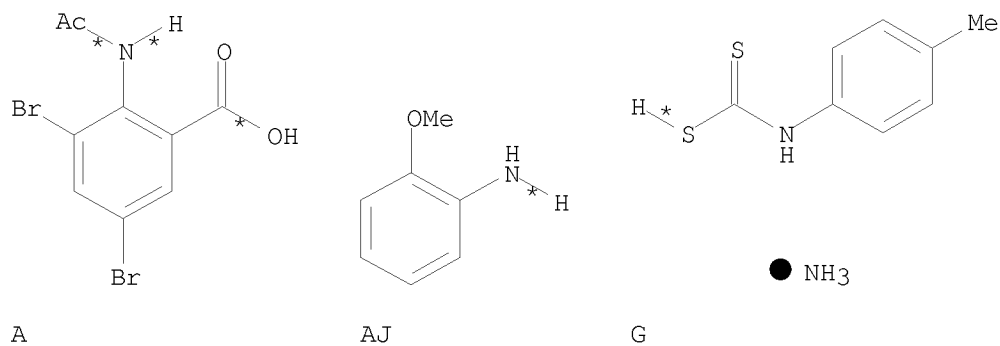


AB

RX(21) RCT A 16610-45-0, AJ 90-04-0  
RGT D 10025-87-3 POC13  
PRO AA 104308-99-8

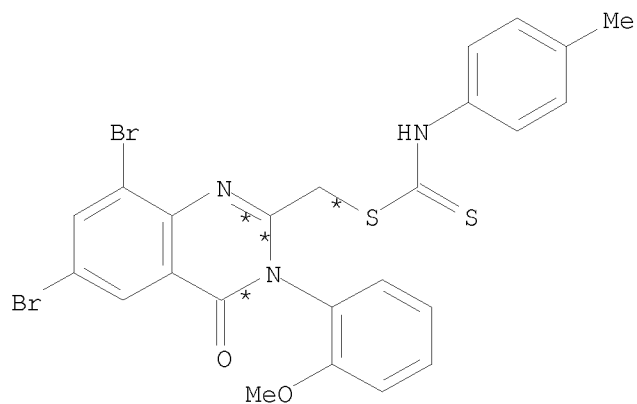
RX(13) RCT AA 104308-99-8, E 1074-52-8  
PRO AB 104308-86-3

RX(34) OF 40 COMPOSED OF RX(21), RX(14)  
RX(34) A + AJ + G ==> AC



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2  
STEPS  
→

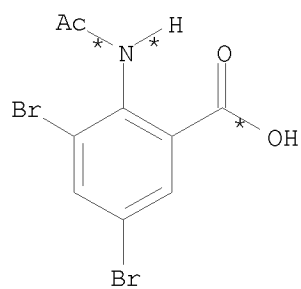


AC

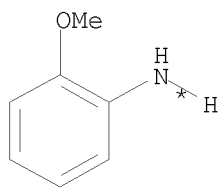
RX(21) RCT A 16610-45-0, AJ 90-04-0  
RGT D 10025-87-3 POC13  
PRO AA 104308-99-8

RX(14) RCT AA 104308-99-8, G 13036-91-4  
PRO AC 104308-87-4

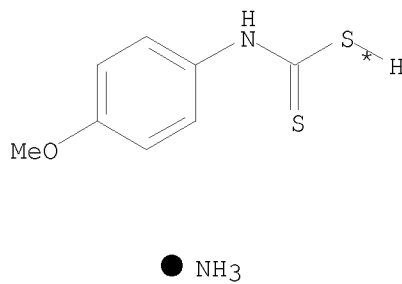
RX(35) OF 40 COMPOSED OF RX(21), RX(15)  
RX(35) A + AJ + I ==> AD



A



AJ

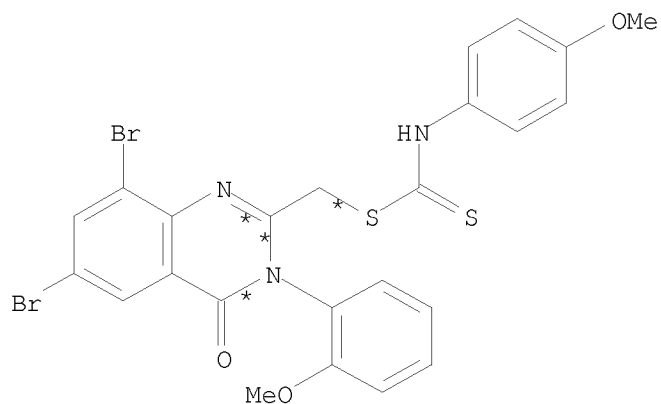


I

2  
STEPS  
→



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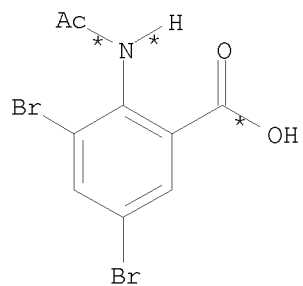


AD

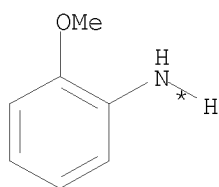
RX(21)      RCT    A 16610-45-0, AJ 90-04-0  
               RGT    D 10025-87-3 POC13  
               PRO    AA 104308-99-8

RX(15)      RCT    AA 104308-99-8, I 15866-98-5  
               PRO    AD 104308-89-6

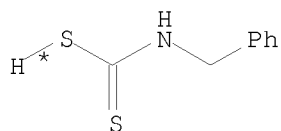
RX(36) OF 40 COMPOSED OF RX(21), RX(16)  
 RX(36)      A    +    AJ    +    K    ==>    AE



A



AJ

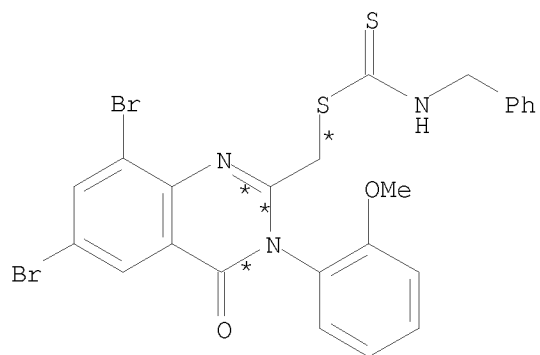


K



2  
 STEPS  
 →

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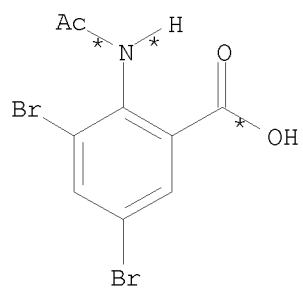


AE

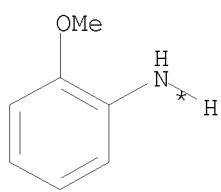
RX(21) RCT A 16610-45-0, AJ 90-04-0  
RGT D 10025-87-3 POC13  
PRO AA 104308-99-8

RX(16) RCT AA 104308-99-8, K 41270-27-3  
PRO AE 104308-90-9

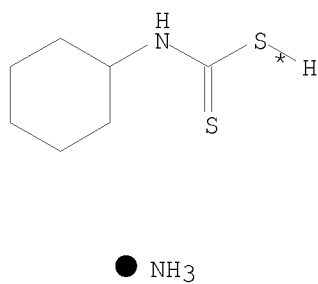
RX(37) OF 40 COMPOSED OF RX(21), RX(17)  
RX(37) A + AJ + M ==> AF



A



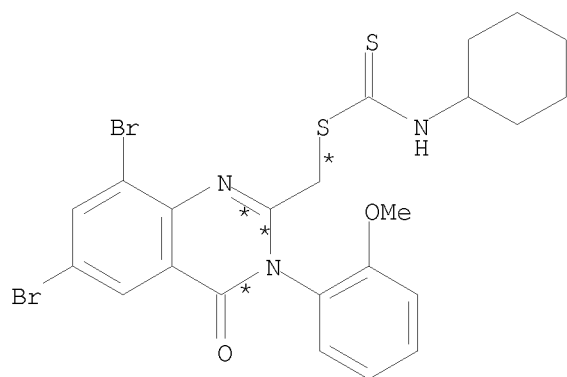
AJ



M

2  
STEPS  
→

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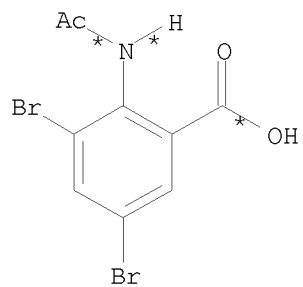


AF

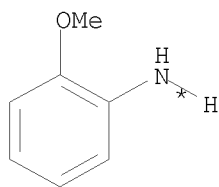
RX(21)      RCT    A 16610-45-0, AJ 90-04-0  
               RGT    D 10025-87-3 POC13  
               PRO    AA 104308-99-8

RX(17)      RCT    AA 104308-99-8, M 66917-87-1  
               PRO    AF 104308-91-0

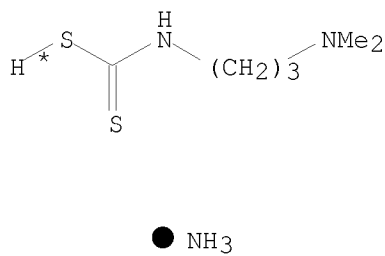
RX(38) OF 40 COMPOSED OF RX(21), RX(18)  
 RX(38)      A    +    AJ    +    O    ==>    AG



A



AJ

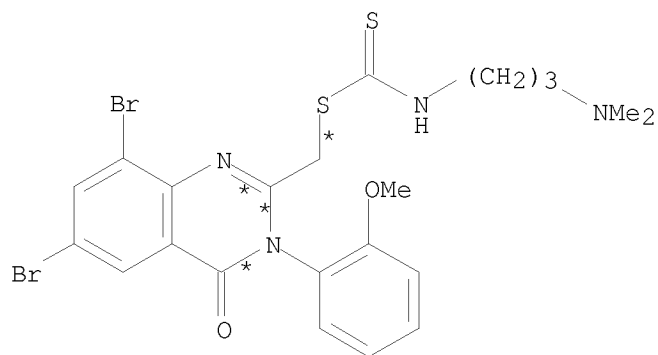


O



2  
 STEPS  
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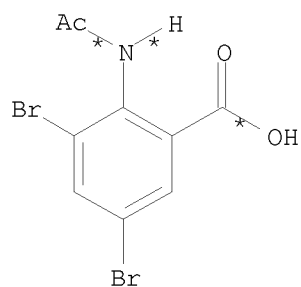


AG

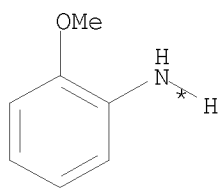
RX(21) RCT A 16610-45-0, AJ 90-04-0  
 RGT D 10025-87-3 POC13  
 PRO AA 104308-99-8

RX(18) RCT AA 104308-99-8, O 200131-07-3  
 PRO AG 104308-92-1

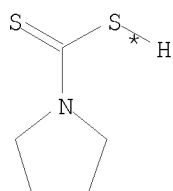
RX(39) OF 40 COMPOSED OF RX(21), RX(19)  
 RX(39) A + AJ + Q ==> AH



A



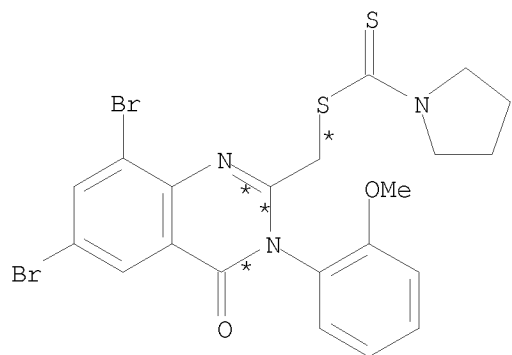
AJ



● NH3  
 Q

2  
 STEPS  
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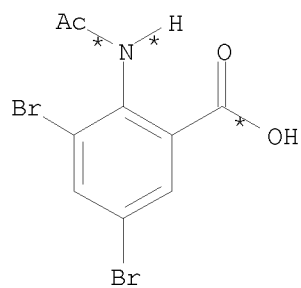


AH

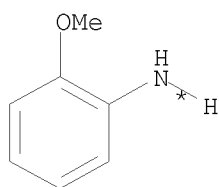
RX(21) RCT A 16610-45-0, AJ 90-04-0  
 RGT D 10025-87-3 POC13  
 PRO AA 104308-99-8

RX(19) RCT AA 104308-99-8, Q 5108-96-3  
 PRO AH 104308-93-2

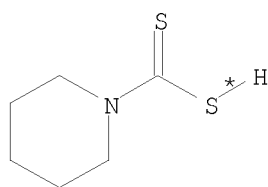
RX(40) OF 40 COMPOSED OF RX(21), RX(20)  
 RX(40) A + AJ + S ==> AI



A



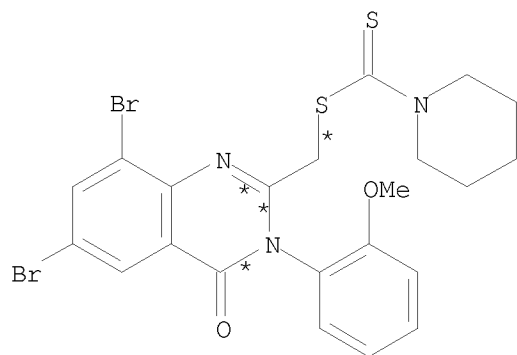
AJ



S

● NH<sub>3</sub>

2  
 STEPS  
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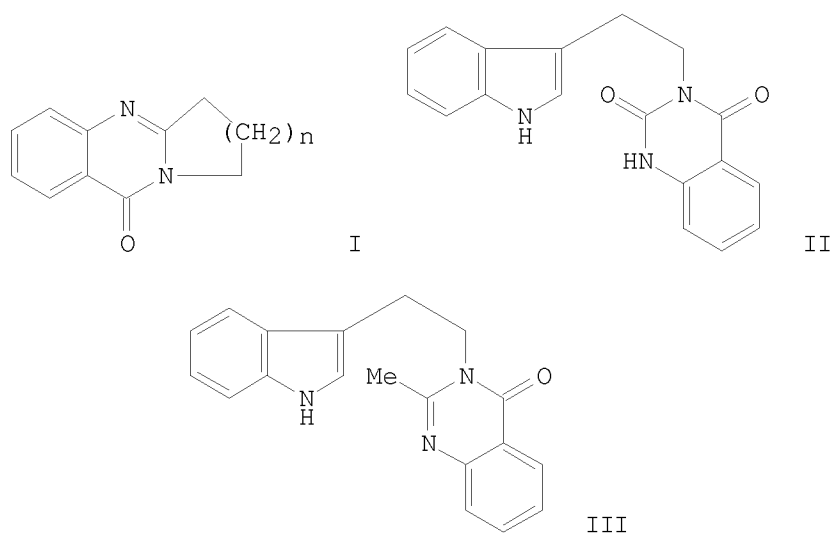


AI

RX(21) RCT A 16610-45-0, AJ 90-04-0  
RGT D 10025-87-3 POC13  
PRO AA 104308-99-8

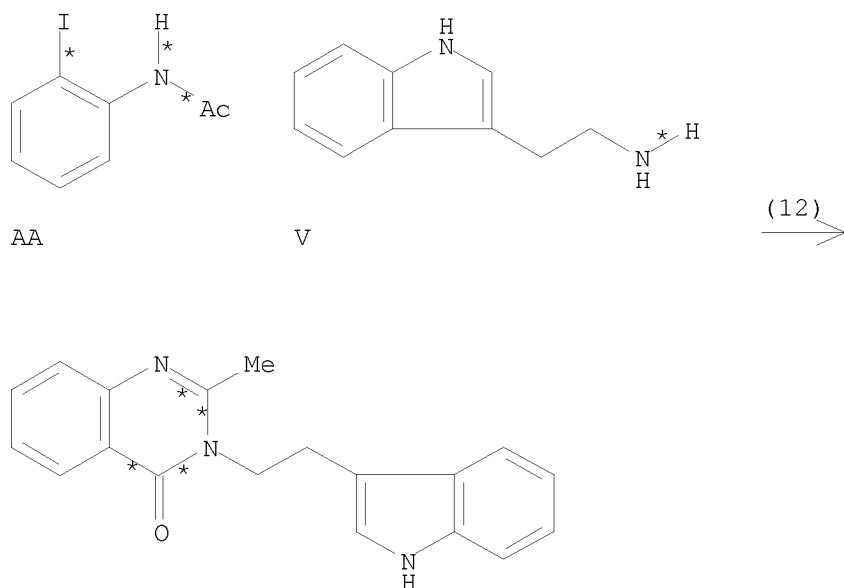
RX(20) RCT AA 104308-99-8, S 49791-55-1  
PRO AI 104308-94-3

L3 ANSWER 193 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 105:97419 CASREACT  
TITLE: One pot synthesis of quinazoline derivatives by use of  
palladium catalyzed carbonylation  
AUTHOR(S): Mori, Miwako; Kobayashi, Hiromi; Kimura, Masaya; Ban,  
Yoshio  
CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, 060, Japan  
SOURCE: Heterocycles (1985), 23(11), 2803-6  
CODEN: HTCYAM; ISSN: 0385-5414  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Quinazolines I ( $n = 1-3$ ) were prepared from a mixture of o-iodoaniline and lactams. Quinazolinones II and III were prepared from acyl-o-iodoanilines and primary amines through the palladium-catalyzed insertion of carbon monoxide. II underwent ring closure to rutecarpine with POC13.

RX(12) OF 22 AA + V ==> AB



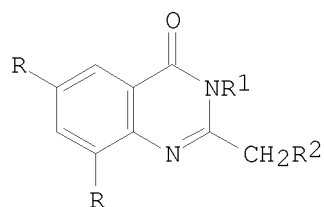
AB

RX(12) RCT AA 19591-17-4, V 61-54-1  
 RGT D 584-08-7 K2CO3, E 630-08-0 CO  
 PRO AB 103970-47-4

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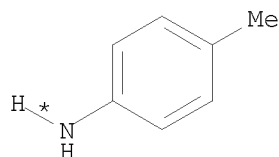
CAT 69058-45-3 Palladium, bis(acetato-κO)(triphenylphosphine)-  
SOL 680-31-9 HMPT

L3 ANSWER 194 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 105:97416 CASREACT  
TITLE: Synthesis and biological activities of certain  
derivatives of 3-aryl-4(3H)-quinazolinones. Part II  
AUTHOR(S): Rao, A. Devender; Shankar, C. Ravi; Reddy, P.  
Bhaghavan; Reddy, V. Malla  
CORPORATE SOURCE: Coll. Pharm. Sci., Kakatiya Univ., Warangal, 506 009,  
India  
SOURCE: Journal of the Indian Chemical Society (1985), 62(3),  
234-7  
CODEN: JICSAH; ISSN: 0019-4522  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



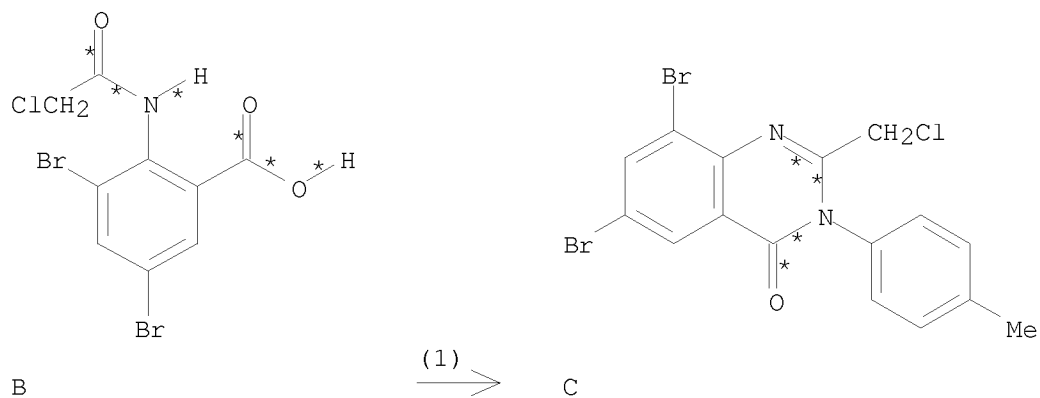
AB 3-Arylquinazolinones I [R = H, Br; R1 = 4-MeC6H4, 2-MeC6H4, 4-O2NC6H4, 2-O2NC6H4; R2 = NMe2, NEt2, N(CH2CH2OH)2, piperidino, morpholino, 4-AcNHC6H4SO2, etc.] were prepared from I (R2 = Cl), which were obtained by cyclocondensation of N-chloroacetylanthranilic acids with R1NH2 in the presence of PCl3. I are antifungal agents, I (R = H, R1 = 4-O2NC6H4, R2 = 4-AcNHC6H4SO2) giving total control of Curvularia lunata and Fusarium oxysporum at 800 µg/mL.

RX(1) OF 61      A + B ==> C...



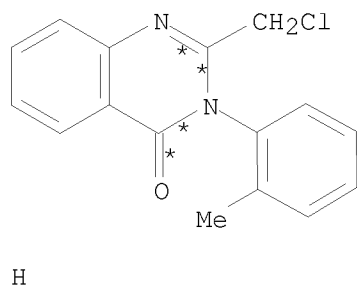
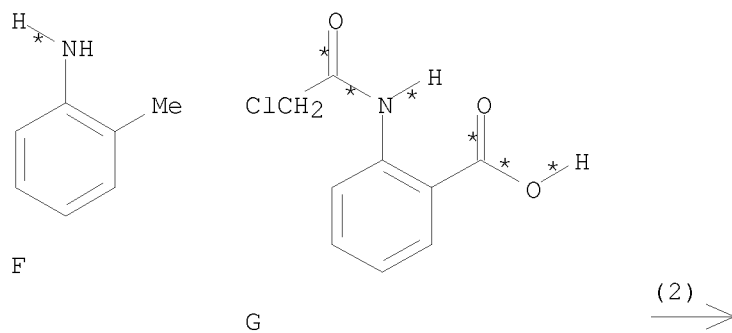


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RX(1)      RCT    A 106-49-0, B 103952-88-1  
               RGT    D 7719-12-2 PC13  
               PRO    C 103952-89-2  
               SOL    108-88-3 PhMe

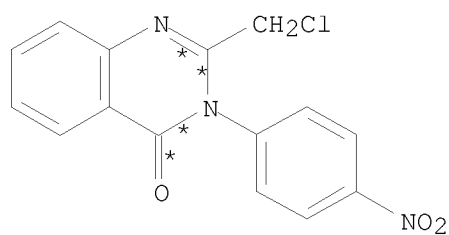
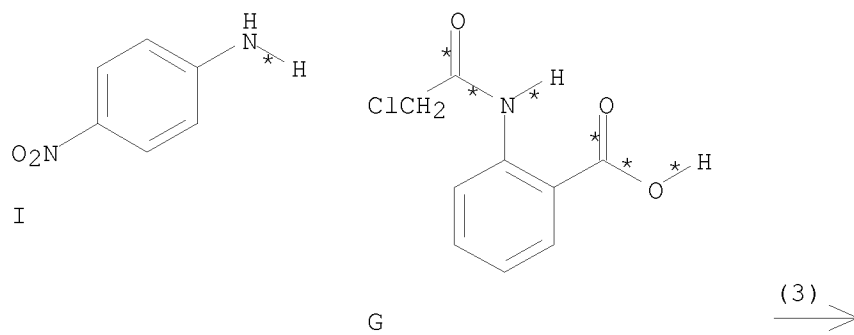
RX(2) OF 61      F + G  $\implies$  H...



RX(2)      RCT    F 95-53-4, G 14422-49-2  
               RGT    D 7719-12-2 PC13  
               PRO    H 3166-54-9  
               SOL    108-88-3 PhMe

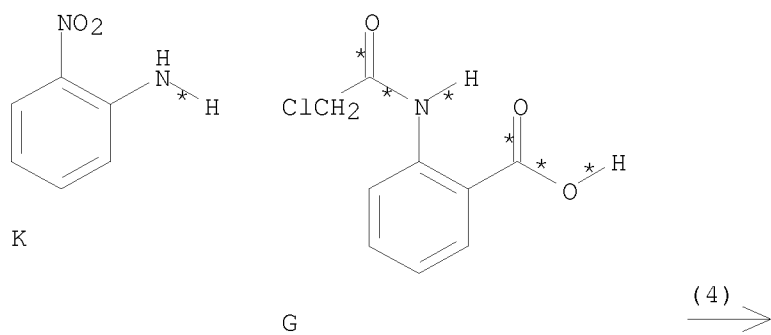
10/ 562,112

RX(3) OF 61      I + G ==> J...

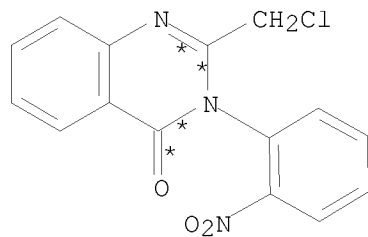


RX(3)      RCT    I 100-01-6, G 14422-49-2  
             RGT    D 7719-12-2 PC13  
             PRO    J 103952-90-5  
             SOL    108-88-3 PhMe

RX(4) OF 61      K + G ==> L...



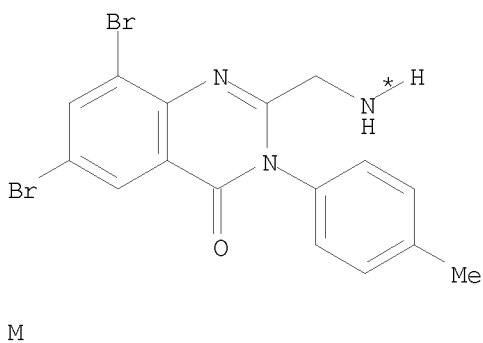
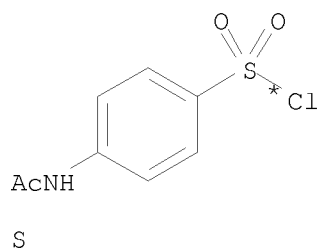
10/ 562,112



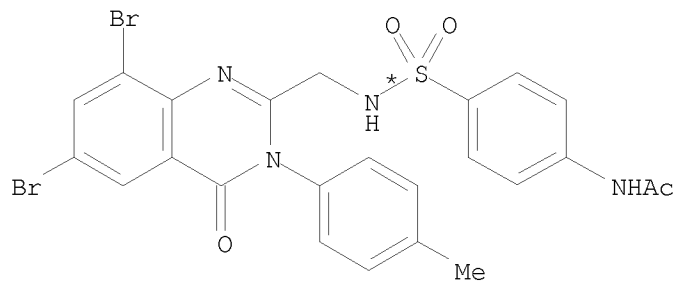
L

RX(4)      RCT    K 88-74-4, G 14422-49-2  
              RGT    D 7719-12-2 PC13  
              PRO    L 80096-22-6  
              SOL    108-88-3 PhMe

RX(9) OF 61      ...S + M ==> T



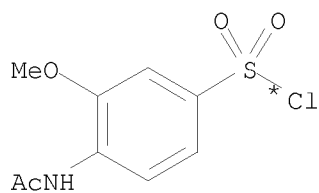
(9) ➞



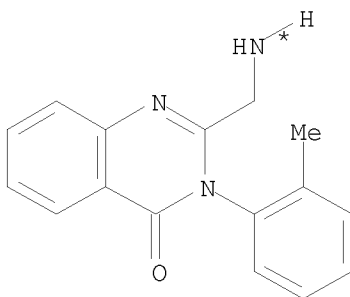
RX(9)      RCT    S 121-60-8, M 103952-91-6  
              PRO    T 103952-99-4  
              SOL    110-86-1 Pyridine

RX(10) OF 61      ...U + P ==> V

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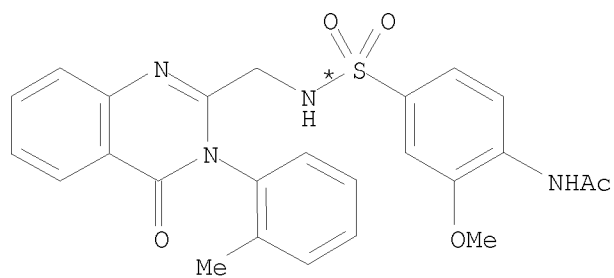


U



P

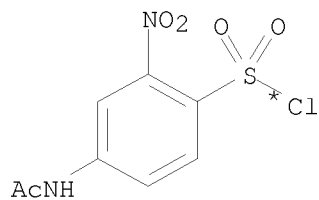
(10)  $\longrightarrow$



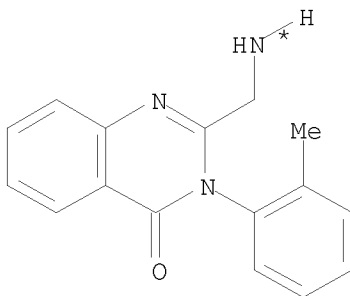
V

RX(10)     RCT   U 46713-94-4, P 80096-33-9  
              PRO   V 103953-04-4  
              SOL   110-86-1 Pyridine

RX(11) OF 61     ...W + P ==> X



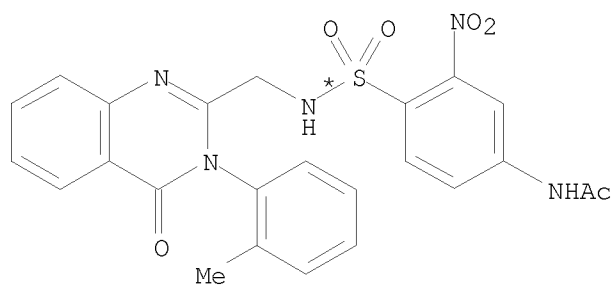
W



P

(11)  $\longrightarrow$

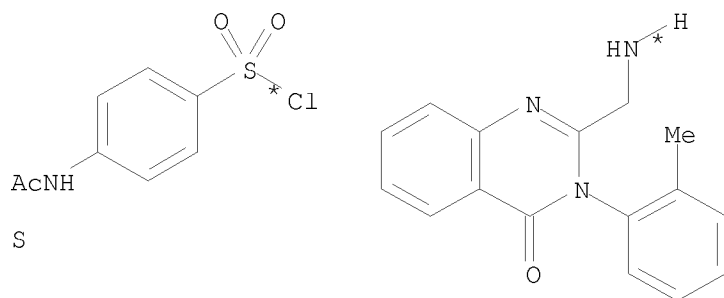
10/ 562,112



X

RX(11) RCT W 19300-50-6, P 80096-33-9  
PRO X 103953-05-5  
SOL 110-86-1 Pyridine

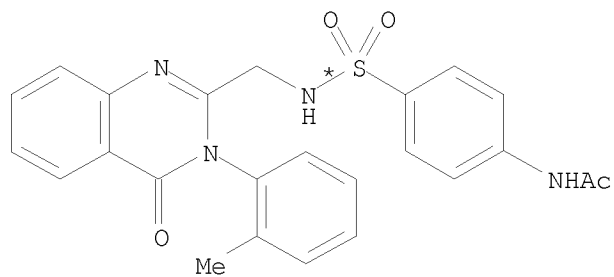
RX(12) OF 61 ...S + P ==> Y



S

P

(12)  $\longrightarrow$

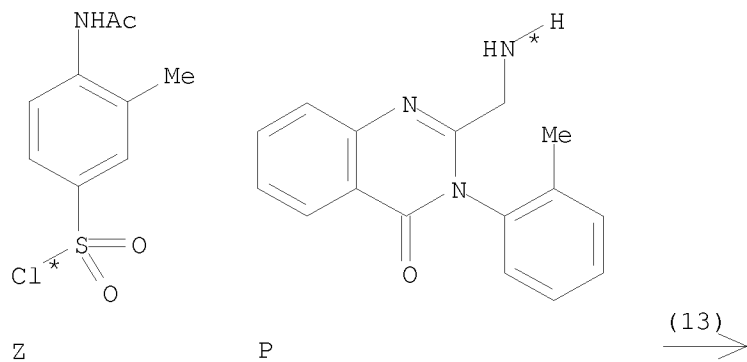


Y

RX(12) RCT S 121-60-8, P 80096-33-9  
PRO Y 103953-06-6  
SOL 110-86-1 Pyridine

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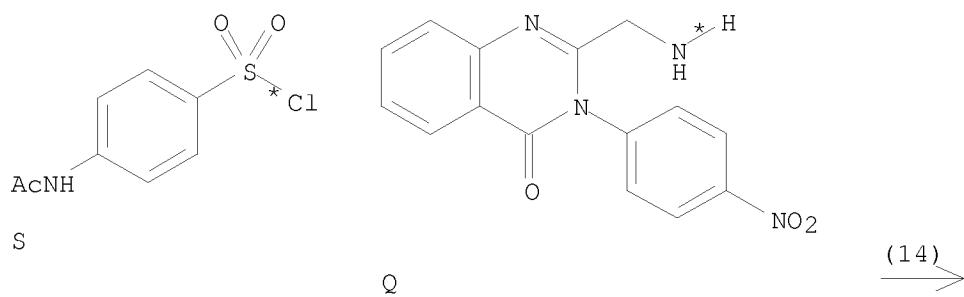
RX(13) OF 61      ...Z + P ==> AA



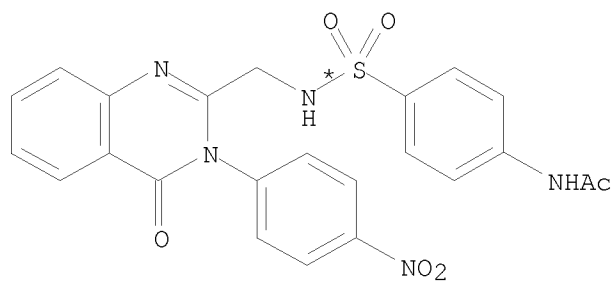
AA

RX(13)      RCT    Z 14988-21-7, P 80096-33-9  
PRO    AA 103953-07-7  
SOL    110-86-1 Pyridine

RX(14) OF 61      ...S + Q ==> AB



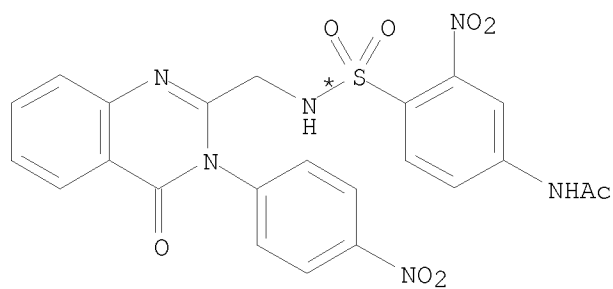
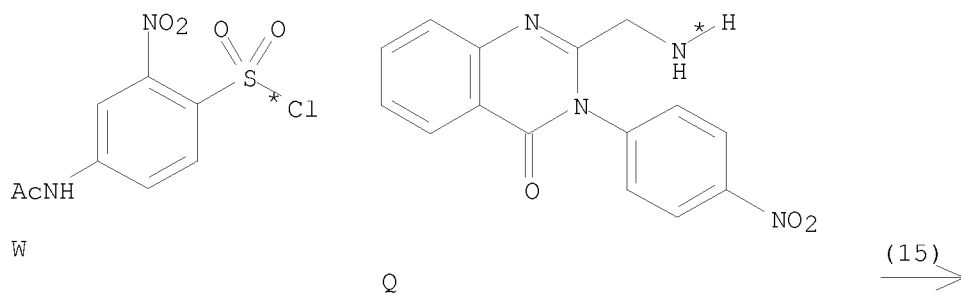
10/ 562,112



AB

RX(14) RCT S 121-60-8, Q 103952-92-7  
PRO AB 103953-00-0  
SOL 110-86-1 Pyridine

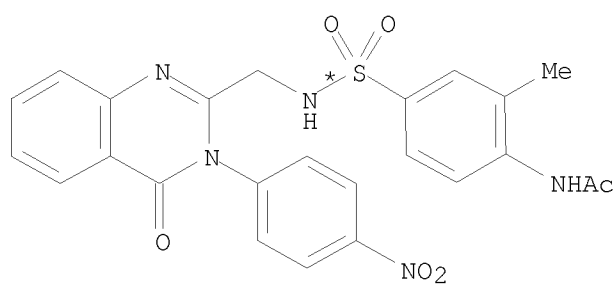
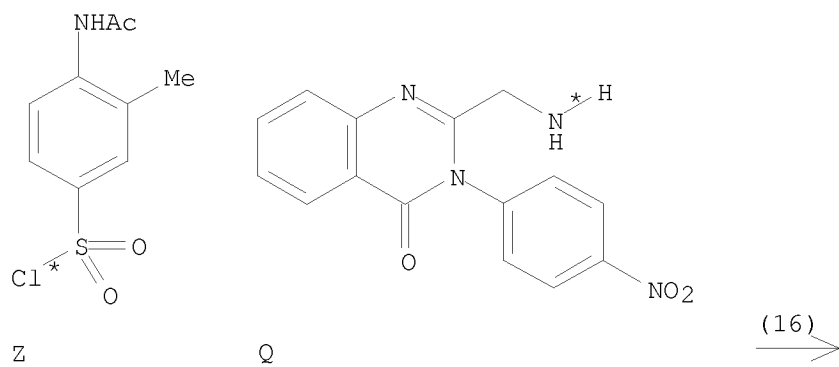
RX(15) OF 61 ...W + Q ==> AC



AC

RX(15) RCT W 19300-50-6, Q 103952-92-7  
PRO AC 103953-01-1  
SOL 110-86-1 Pyridine

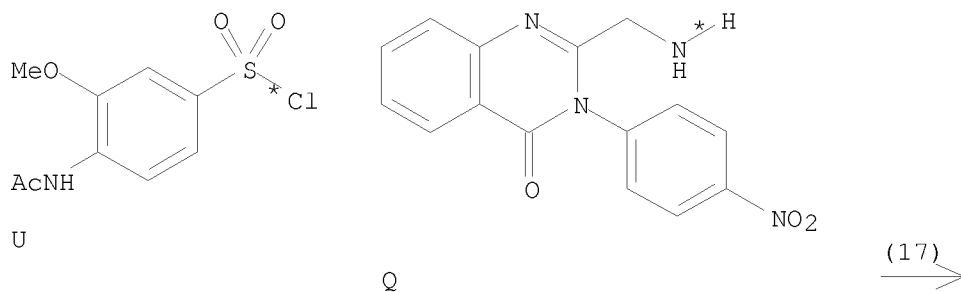
RX(16) OF 61 ...Z + Q ==> AD



AD

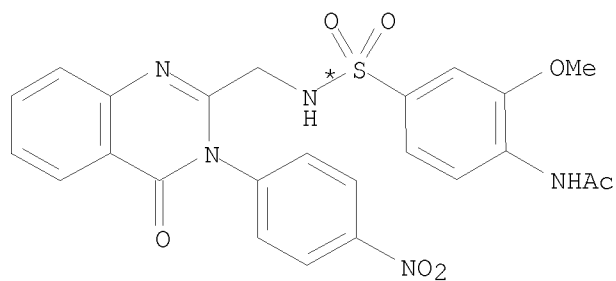
RX(16) RCT Z 14988-21-7, Q 103952-92-7  
 PRO AD 103953-02-2  
 SOL 110-86-1 Pyridine

RX(17) OF 61 ...U + Q ==> AE





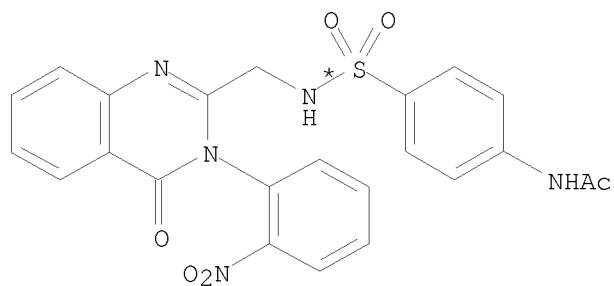
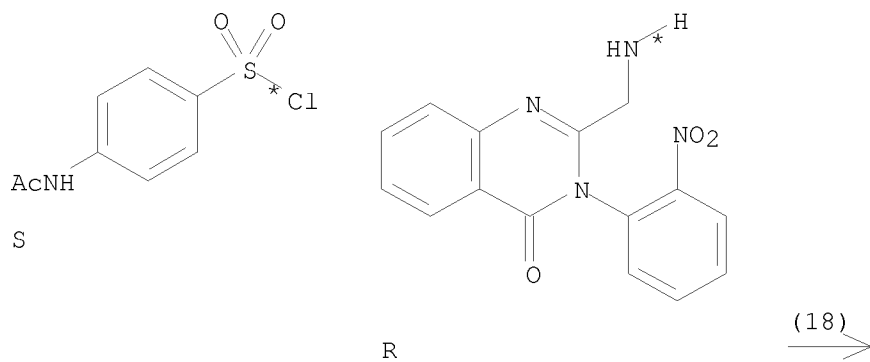
10/ 562,112



AE

RX(17) RCT U 46713-94-4, Q 103952-92-7  
 PRO AE 103953-03-3  
 SOL 110-86-1 Pyridine

RX(18) OF 61 ...S + R ==> AF

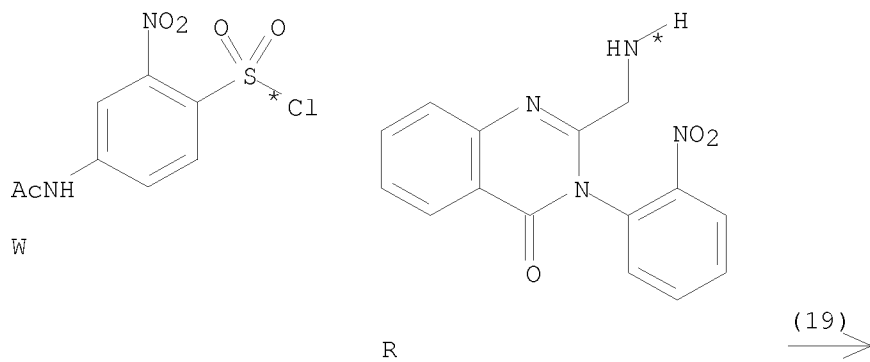


AF

RX(18) RCT S 121-60-8, R 103952-93-8  
 PRO AF 103953-08-8  
 SOL 110-86-1 Pyridine

10/ 562,112

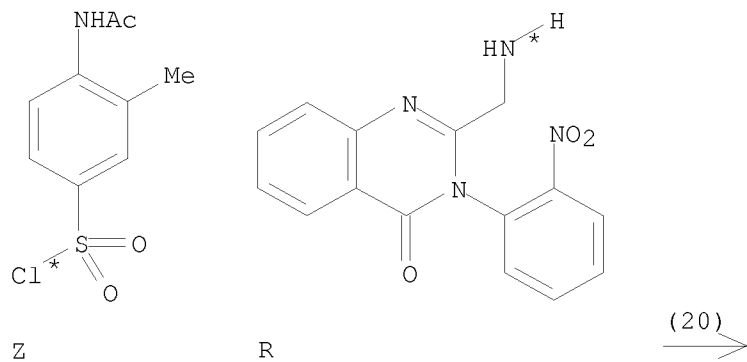
RX(19) OF 61      ...W + R ==> AG



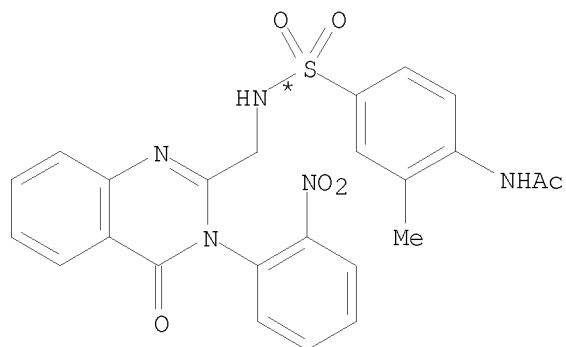
AG

RX(19)      RCT    W 19300-50-6, R 103952-93-8  
             PRO    AG 103953-09-9  
             SOL    110-86-1 Pyridine

RX(20) OF 61      ...Z + R ==> AH



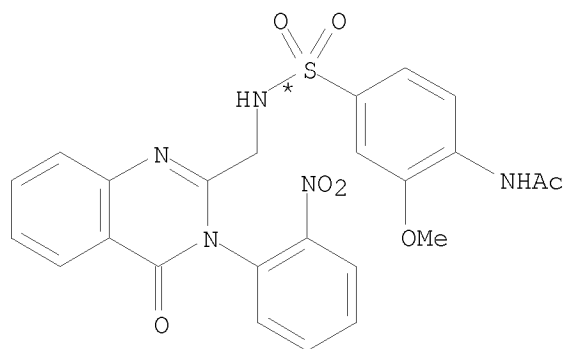
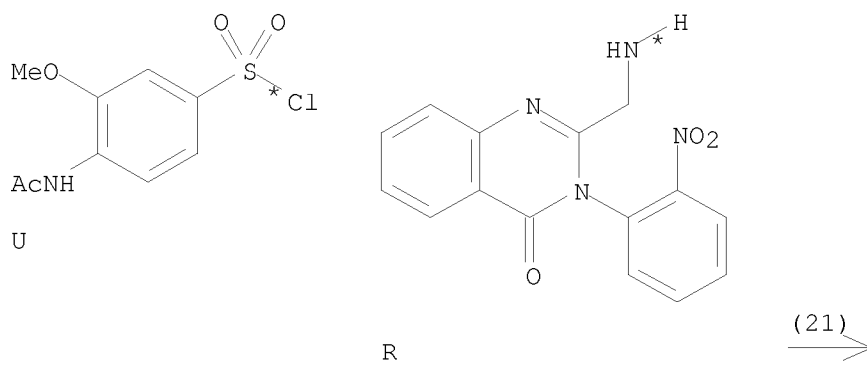
10/ 562,112



AH

RX(20) RCT Z 14988-21-7, R 103952-93-8  
PRO AH 103953-10-2  
SOL 110-86-1 Pyridine

RX(21) OF 61 ...U + R ==> AI



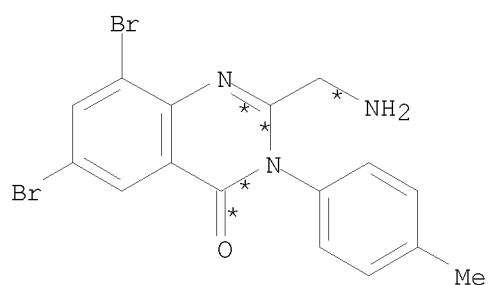
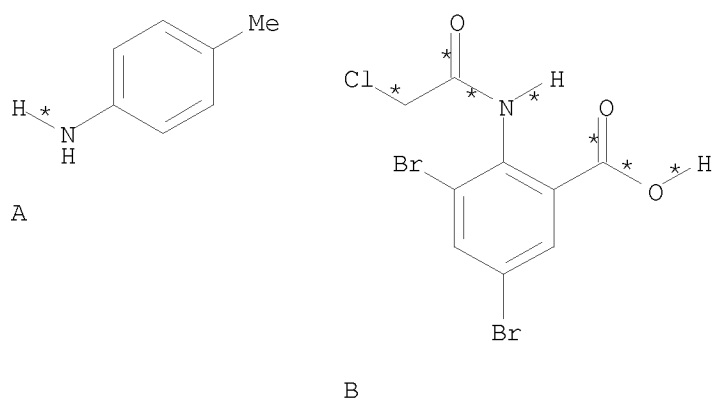
AI

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RX(21) RCT U 46713-94-4, R 103952-93-8  
PRO AI 103953-11-3  
SOL 110-86-1 Pyridine

RX(27) OF 61 COMPOSED OF RX(1), RX(5)

RX(27) A + B ==> M



M

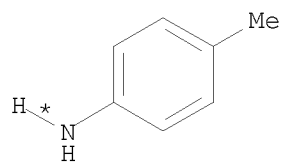
RX(1) RCT A 106-49-0, B 103952-88-1  
RGT D 7719-12-2 PC13  
PRO C 103952-89-2  
SOL 108-88-3 PhMe

RX(5) RCT C 103952-89-2  
RGT N 7664-41-7 NH3  
PRO M 103952-91-6  
SOL 110-86-1 Pyridine

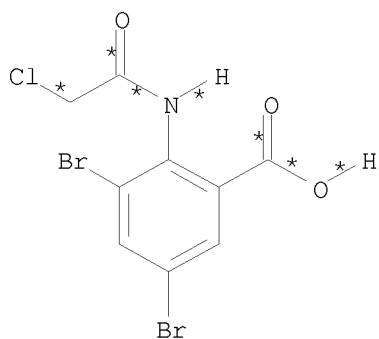
RX(28) OF 61 COMPOSED OF RX(1), RX(22)

RX(28) A + B + AJ ==> AK

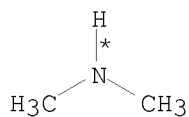
10/ 562,112



A

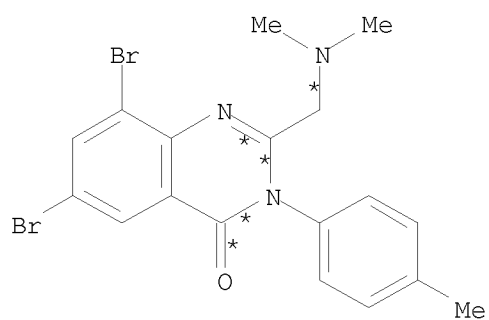


B



AJ

2  
STEPS  
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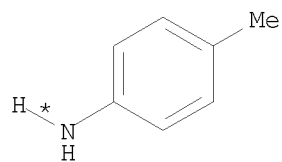
AK

RX(1) RCT A 106-49-0, B 103952-88-1  
RGT D 7719-12-2 PC13  
PRO C 103952-89-2  
SOL 108-88-3 PhMe

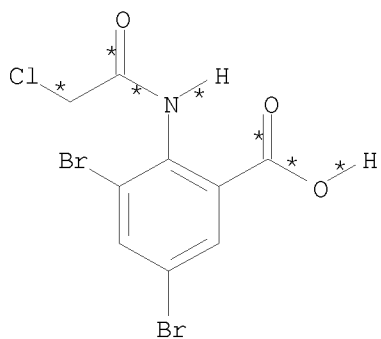
RX(22) RCT C 103952-89-2, AJ 124-40-3  
PRO AK 103952-94-9  
SOL 110-86-1 Pyridine

RX(29) OF 61 COMPOSED OF RX(1), RX(23)  
RX(29) A + B + AL ==> AM

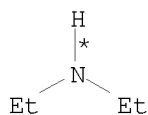
10/ 562,112



A

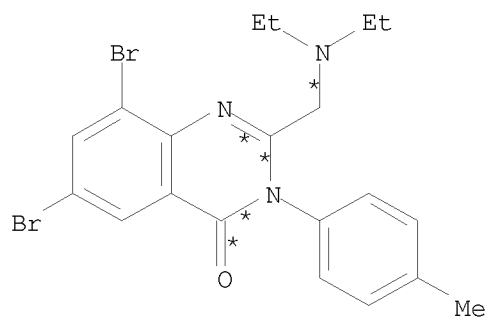


B



AL

2  
STEPS  
→



AM

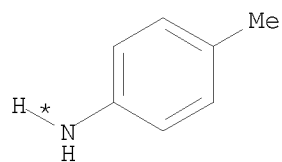
RX(1) RCT A 106-49-0, B 103952-88-1  
RGT D 7719-12-2 PC13  
PRO C 103952-89-2  
SOL 108-88-3 PhMe

RX(23) RCT C 103952-89-2, AL 109-89-7  
PRO AM 103952-95-0  
SOL 110-86-1 Pyridine

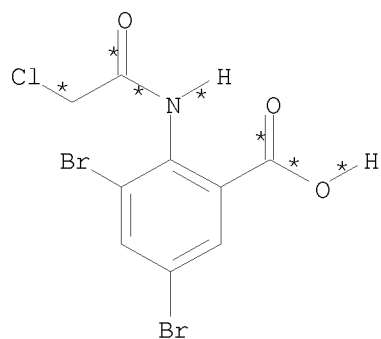
RX(30) OF 61 COMPOSED OF RX(1), RX(24)

RX(30) A + B + AN ==> AO

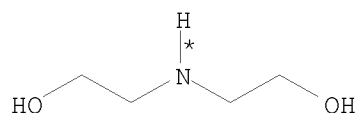
10/ 562,112



A

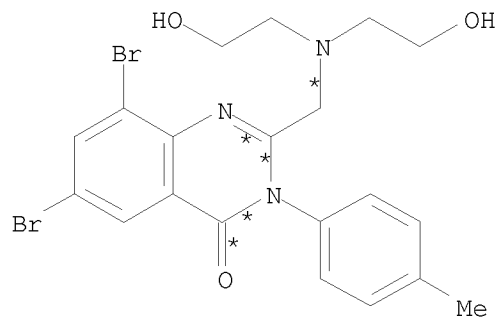


B



AN

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STEPS  
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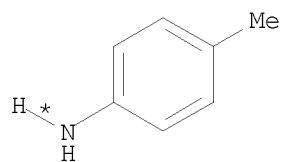
AO

RX(1) RCT A 106-49-0, B 103952-88-1  
RGT D 7719-12-2 PC13  
PRO C 103952-89-2  
SOL 108-88-3 PhMe

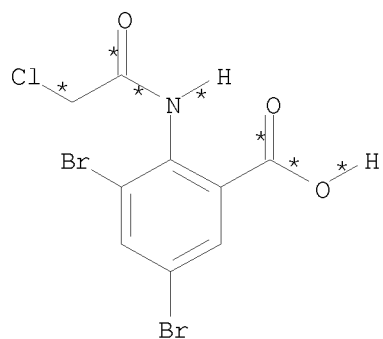
RX(24) RCT C 103952-89-2, AN 111-42-2  
PRO AO 103952-96-1  
SOL 110-86-1 Pyridine

RX(31) OF 61 COMPOSED OF RX(1), RX(25)  
RX(31) A + B + AP ==> AQ

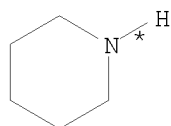
10/ 562,112



A

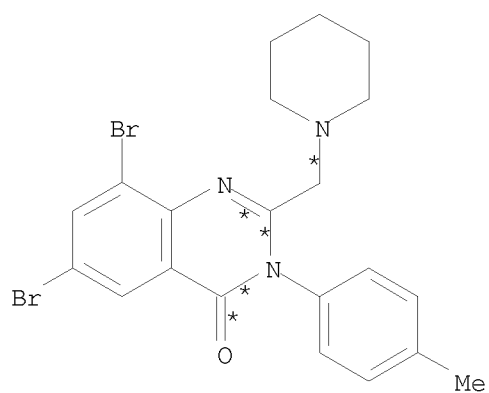


B



AP

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STEPS  
→



AQ

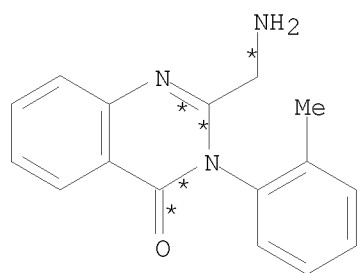
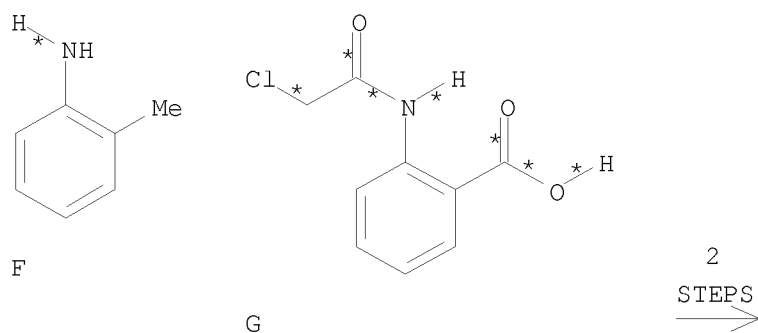
RX(1) RCT A 106-49-0, B 103952-88-1  
RGT D 7719-12-2 PC13  
PRO C 103952-89-2  
SOL 108-88-3 PhMe

RX(25) RCT C 103952-89-2, AP 110-89-4  
PRO AQ 103952-97-2  
SOL 110-86-1 Pyridine

RX(33) OF 61 COMPOSED OF RX(2), RX(6)  
RX(33) F + G ==> P



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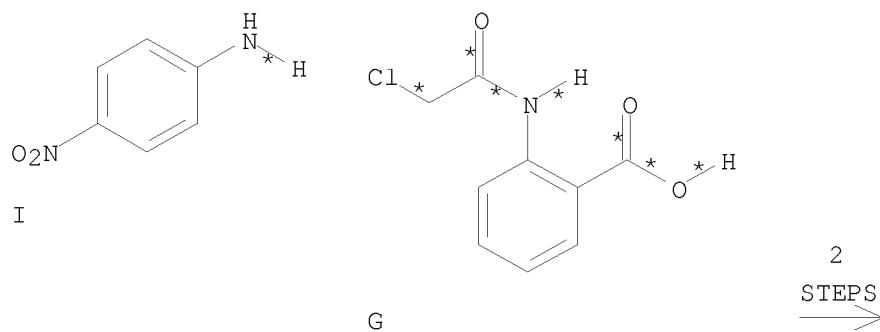
P

RX(2)      RCT    F 95-53-4, G 14422-49-2  
              RGT    D 7719-12-2 PC13  
              PRO    H 3166-54-9  
              SOL    108-88-3 PhMe

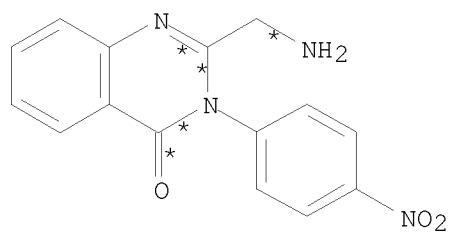
RX(6)      RCT    H 3166-54-9  
              RGT    N 7664-41-7 NH3  
              PRO    P 80096-33-9  
              SOL    110-86-1 Pyridine

RX(34) OF 61 COMPOSED OF RX(3), RX(7)

RX(34)      I    +    G    ==>    Q



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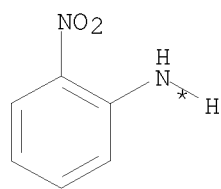
Q

RX(3)      RCT    I 100-01-6, G 14422-49-2  
              RGT    D 7719-12-2 PC13  
              PRO    J 103952-90-5  
              SOL    108-88-3 PhMe

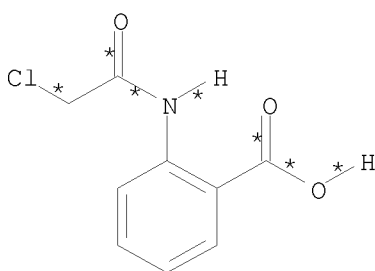
RX(7)      RCT    J 103952-90-5  
              RGT    N 7664-41-7 NH3  
              PRO    Q 103952-92-7  
              SOL    110-86-1 Pyridine

RX(35) OF 61 COMPOSED OF RX(4), RX(8)

RX(35)      K    +    G    ==>    R

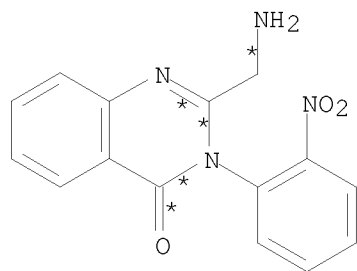


K



G

2  
 STEPS  
 →



R

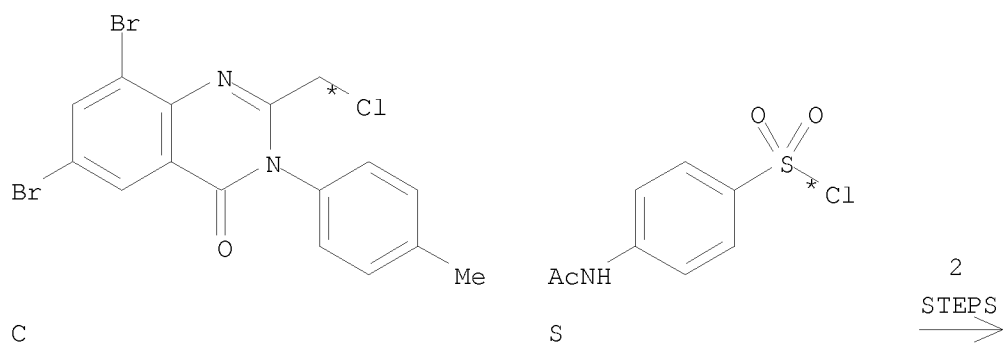
10/ 562,112

RX(4) RCT K 88-74-4, G 14422-49-2  
RGT D 7719-12-2 PC13  
PRO L 80096-22-6  
SOL 108-88-3 PhMe

RX(8) RCT L 80096-22-6  
RGT N 7664-41-7 NH3  
PRO R 103952-93-8  
SOL 110-86-1 Pyridine

RX(36) OF 61 COMPOSED OF RX(5), RX(9)

RX(36) C + S ==> T



T

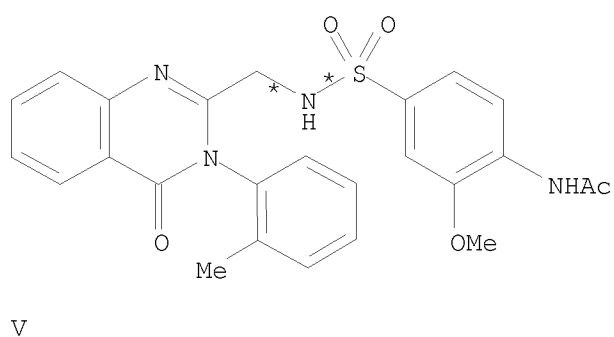
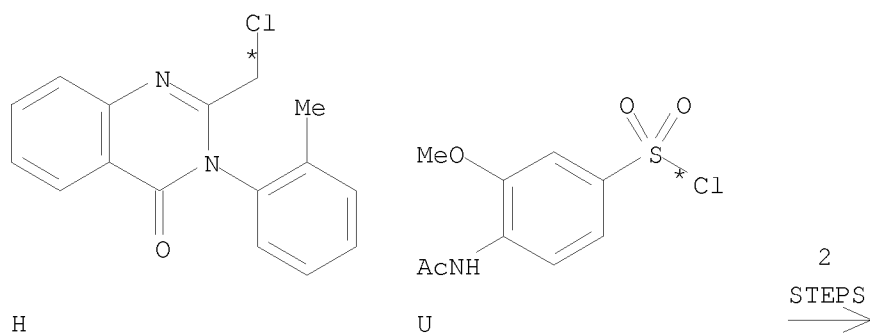
RX(5) RCT C 103952-89-2  
RGT N 7664-41-7 NH3  
PRO M 103952-91-6  
SOL 110-86-1 Pyridine

RX(9) RCT S 121-60-8, M 103952-91-6  
PRO T 103952-99-4  
SOL 110-86-1 Pyridine

RX(37) OF 61 COMPOSED OF RX(6), RX(10)

RX(37) H + U ==> V

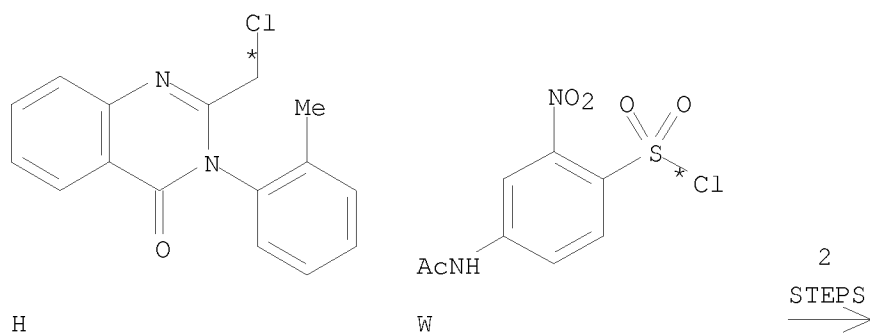
10/ 562,112



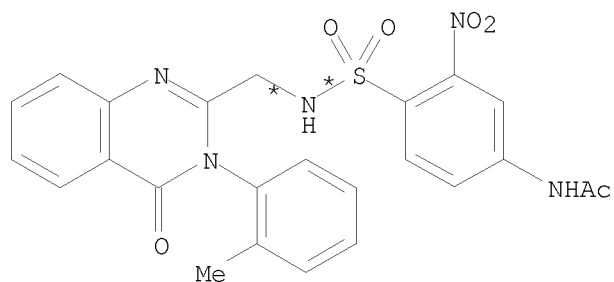
RX(6)      RCT    H 3166-54-9  
              RGT    N 7664-41-7 NH3  
              PRO    P 80096-33-9  
              SOL    110-86-1 Pyridine

RX(10)      RCT    U 46713-94-4, P 80096-33-9  
              PRO    V 103953-04-4  
              SOL    110-86-1 Pyridine

RX(38) OF 61 COMPOSED OF RX(6), RX(11)  
 RX(38)      H    +    W    ==>    X



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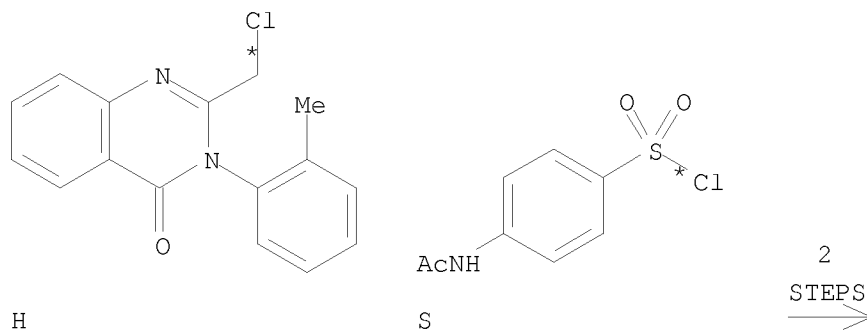


X

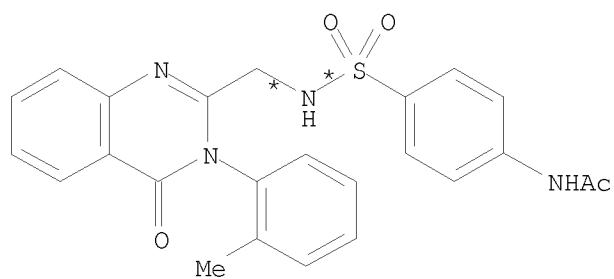
RX(6)      RCT   H 3166-54-9  
             RGT   N 7664-41-7 NH3  
             PRO   P 80096-33-9  
             SOL   110-86-1 Pyridine

RX(11)      RCT   W 19300-50-6, P 80096-33-9  
             PRO   X 103953-05-5  
             SOL   110-86-1 Pyridine

RX(39) OF 61 COMPOSED OF RX(6), RX(12)  
RX(39)      H   +   S   ==>   Y



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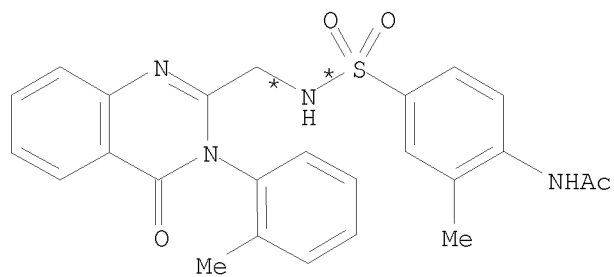
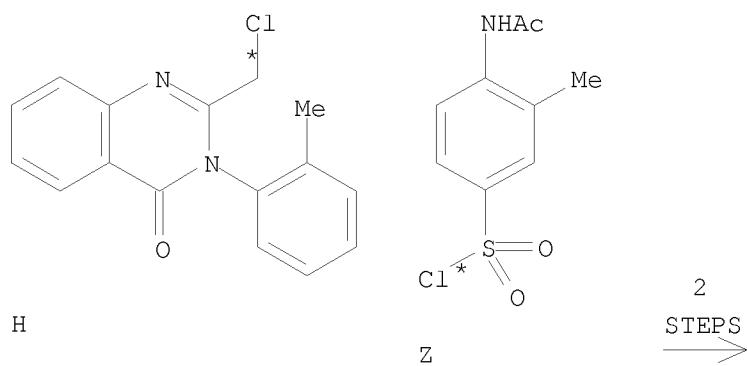


Y

RX(6) RCT H 3166-54-9  
 RGT N 7664-41-7 NH3  
 PRO P 80096-33-9  
 SOL 110-86-1 Pyridine

RX(12) RCT S 121-60-8, P 80096-33-9  
 PRO Y 103953-06-6  
 SOL 110-86-1 Pyridine

RX(40) OF 61 COMPOSED OF RX(6), RX(13)  
 RX(40) H + Z ==> AA



AA

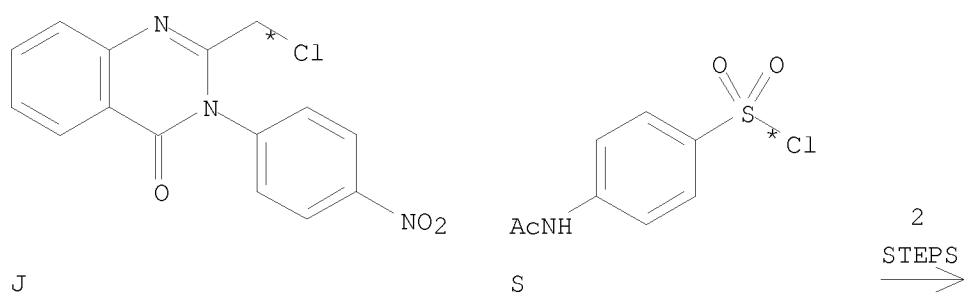
10/ 562,112

RX(6)      RCT   H 3166-54-9  
             RGT   N 7664-41-7 NH3  
             PRO   P 80096-33-9  
             SOL   110-86-1 Pyridine

RX(13)     RCT   Z 14988-21-7, P 80096-33-9  
             PRO   AA 103953-07-7  
             SOL   110-86-1 Pyridine

RX(41) OF 61 COMPOSED OF RX(7), RX(14)

RX(41)      J   +   S   ==>   AB



AB

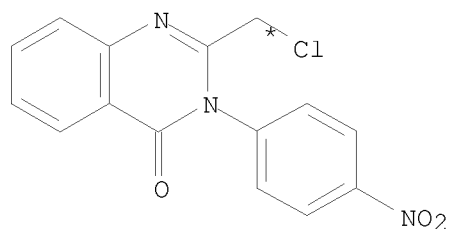
RX(7)      RCT   J 103952-90-5  
             RGT   N 7664-41-7 NH3  
             PRO   Q 103952-92-7  
             SOL   110-86-1 Pyridine

RX(14)     RCT   S 121-60-8, Q 103952-92-7  
             PRO   AB 103953-00-0  
             SOL   110-86-1 Pyridine

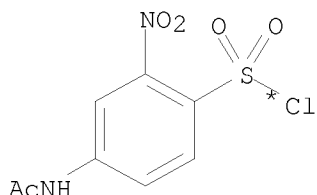
RX(42) OF 61 COMPOSED OF RX(7), RX(15)

RX(42)      J   +   W   ==>   AC

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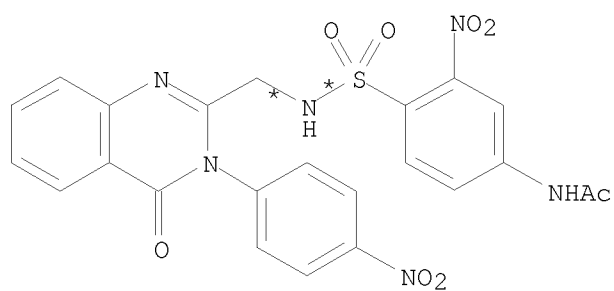


J



W

2  
STEPS  
→

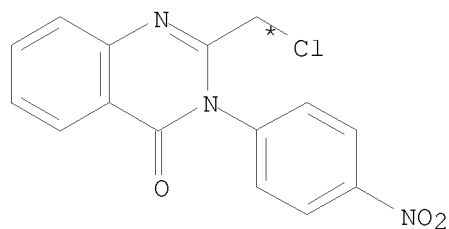


AC

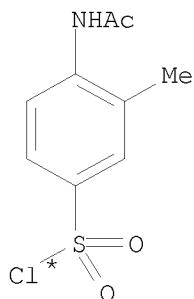
RX(7)      RCT    J 103952-90-5  
              RGT    N 7664-41-7 NH3  
              PRO    Q 103952-92-7  
              SOL    110-86-1 Pyridine

RX(15)      RCT    W 19300-50-6, Q 103952-92-7  
              PRO    AC 103953-01-1  
              SOL    110-86-1 Pyridine

RX(43) OF 61 COMPOSED OF RX(7), RX(16)  
 RX(43)      J    +    Z    ==>    AD



J

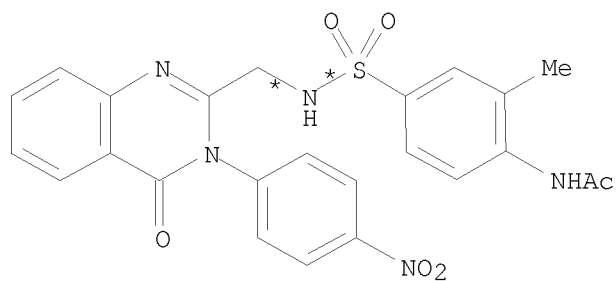


Z

2  
STEPS  
→



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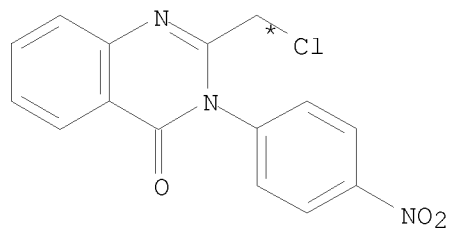
AD

RX(7) RCT J 103952-90-5  
RGT N 7664-41-7 NH3  
PRO Q 103952-92-7  
SOL 110-86-1 Pyridine

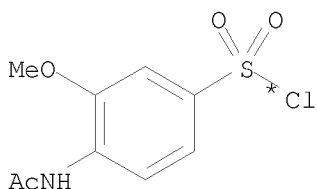
RX(16) RCT Z 14988-21-7, Q 103952-92-7  
PRO AD 103953-02-2  
SOL 110-86-1 Pyridine

RX(44) OF 61 COMPOSED OF RX(7), RX(17)

RX(44) J + U ==> AE

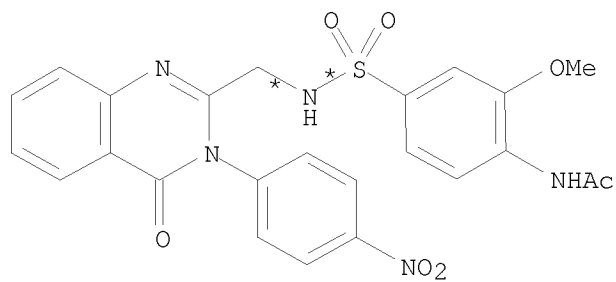


J



U

2  
STEPS  
→



AE

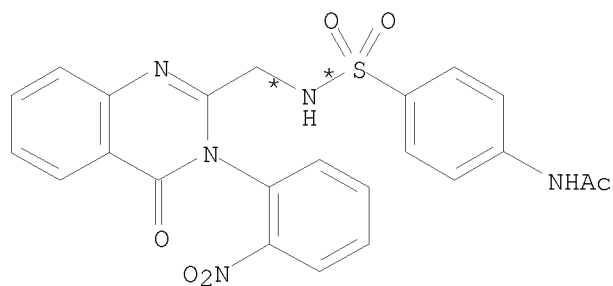
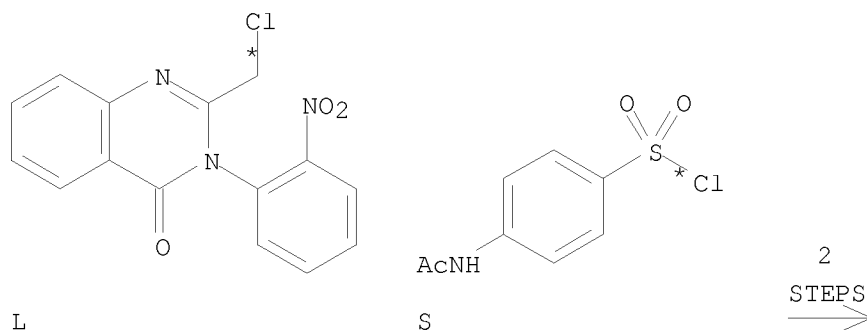
RX(7) RCT J 103952-90-5

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RGT N 7664-41-7 NH3  
PRO Q 103952-92-7  
SOL 110-86-1 Pyridine

RX(17) RCT U 46713-94-4, Q 103952-92-7  
PRO AE 103953-03-3  
SOL 110-86-1 Pyridine

RX(45) OF 61 COMPOSED OF RX(8), RX(18)  
RX(45) L + S ==> AF



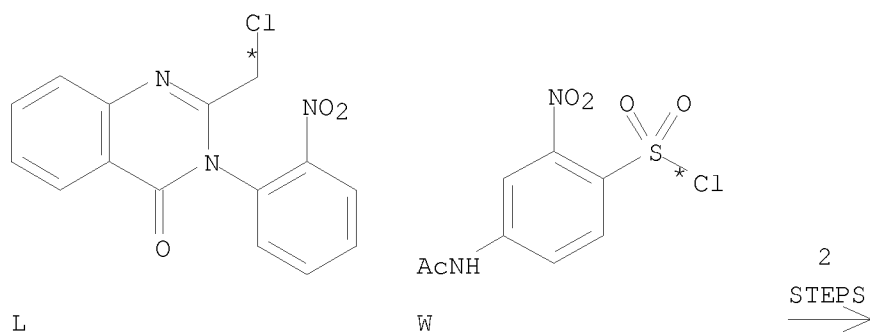
AF

RX(8) RCT L 80096-22-6  
RGT N 7664-41-7 NH3  
PRO R 103952-93-8  
SOL 110-86-1 Pyridine

RX(18) RCT S 121-60-8, R 103952-93-8  
PRO AF 103953-08-8  
SOL 110-86-1 Pyridine

RX(46) OF 61 COMPOSED OF RX(8), RX(19)  
RX(46) L + W ==> AG

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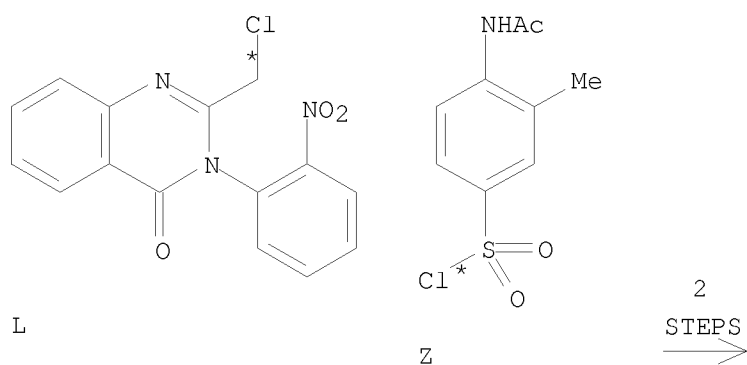


AG

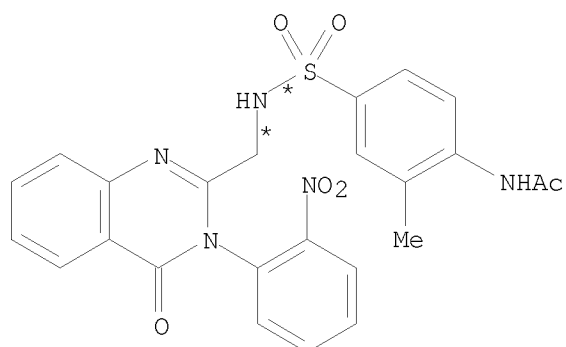
RX(8) RCT L 80096-22-6  
 RGT N 7664-41-7 NH<sub>3</sub>  
 PRO R 103952-93-8  
 SOL 110-86-1 Pyridine

RX(19) RCT W 19300-50-6, R 103952-93-8  
 PRO AG 103953-09-9  
 SOL 110-86-1 Pyridine

RX(47) OF 61 COMPOSED OF RX(8), RX(20)  
 RX(47) L + Z ==> AH



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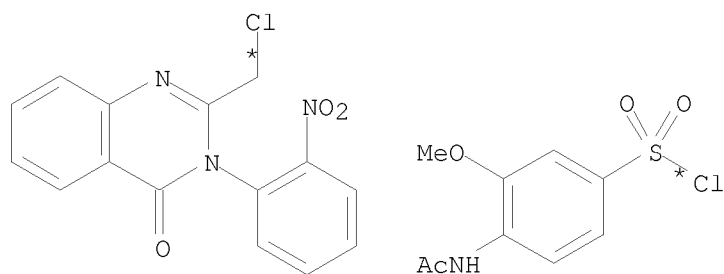


AH

RX(8) RCT L 80096-22-6  
RGT N 7664-41-7 NH3  
PRO R 103952-93-8  
SOL 110-86-1 Pyridine

RX(20) RCT Z 14988-21-7, R 103952-93-8  
PRO AH 103953-10-2  
SOL 110-86-1 Pyridine

RX(48) OF 61 COMPOSED OF RX(8), RX(21)  
RX(48) L + U ==> AI

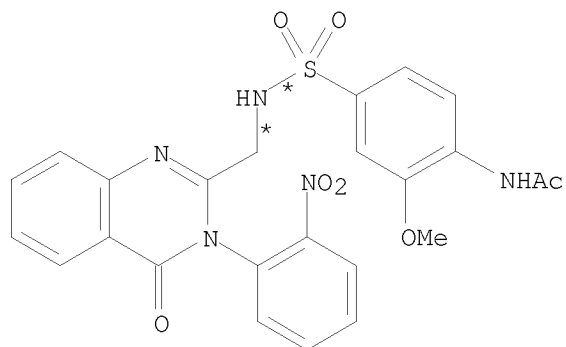


L

U

2  
STEPS  
→

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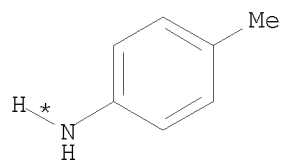


AI

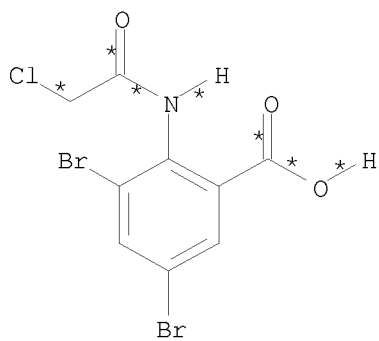
RX(8) RCT L 80096-22-6  
 RGT N 7664-41-7 NH3  
 PRO R 103952-93-8  
 SOL 110-86-1 Pyridine

RX(21) RCT U 46713-94-4, R 103952-93-8  
 PRO AI 103953-11-3  
 SOL 110-86-1 Pyridine

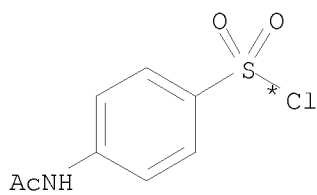
RX(49) OF 61 COMPOSED OF RX(1), RX(5), RX(9)  
 RX(49) A + B + S ==> T



A



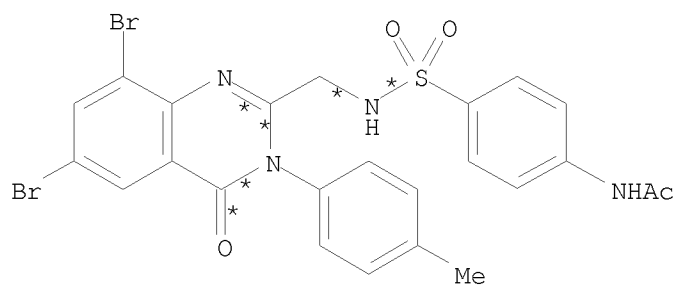
B



S

3  
 STEPS  
 →

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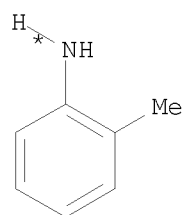
T

RX(1) RCT A 106-49-0, B 103952-88-1  
 RGT D 7719-12-2 PC13  
 PRO C 103952-89-2  
 SOL 108-88-3 PhMe

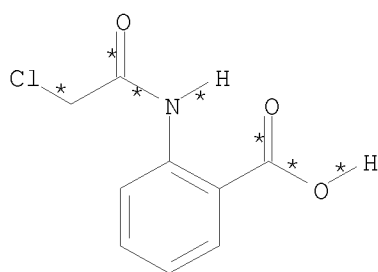
RX(5) RCT C 103952-89-2  
 RGT N 7664-41-7 NH3  
 PRO M 103952-91-6  
 SOL 110-86-1 Pyridine

RX(9) RCT S 121-60-8, M 103952-91-6  
 PRO T 103952-99-4  
 SOL 110-86-1 Pyridine

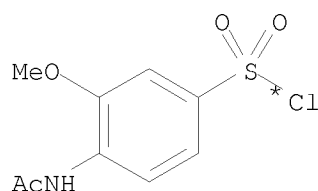
RX(50) OF 61 COMPOSED OF RX(2), RX(6), RX(10)  
 RX(50) F + G + U ==> V



F



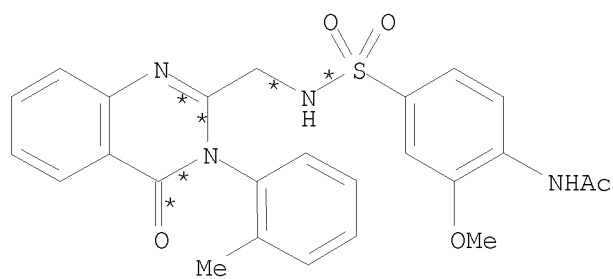
G



U

3  
 STEPS

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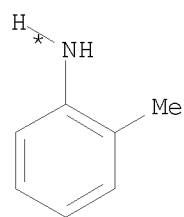
V

RX(2) RCT F 95-53-4, G 14422-49-2  
RGT D 7719-12-2 PC13  
PRO H 3166-54-9  
SOL 108-88-3 PhMe

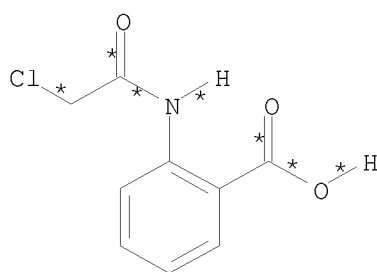
RX(6) RCT H 3166-54-9  
RGT N 7664-41-7 NH3  
PRO P 80096-33-9  
SOL 110-86-1 Pyridine

RX(10) RCT U 46713-94-4, P 80096-33-9  
PRO V 103953-04-4  
SOL 110-86-1 Pyridine

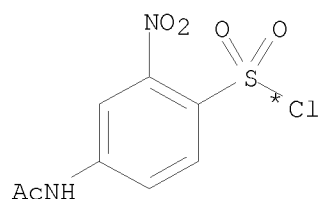
RX(51) OF 61 COMPOSED OF RX(2), RX(6), RX(11)  
RX(51) F + G + W ==> X



F



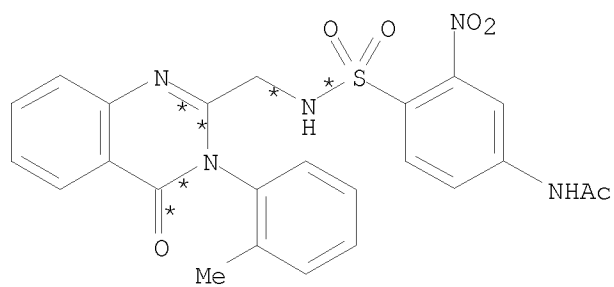
G



W

3  
STEPS  
→

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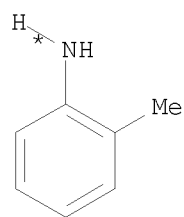
X

RX(2) RCT F 95-53-4, G 14422-49-2  
 RGT D 7719-12-2 PC13  
 PRO H 3166-54-9  
 SOL 108-88-3 PhMe

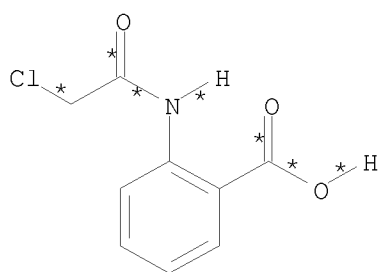
RX(6) RCT H 3166-54-9  
 RGT N 7664-41-7 NH3  
 PRO P 80096-33-9  
 SOL 110-86-1 Pyridine

RX(11) RCT W 19300-50-6, P 80096-33-9  
 PRO X 103953-05-5  
 SOL 110-86-1 Pyridine

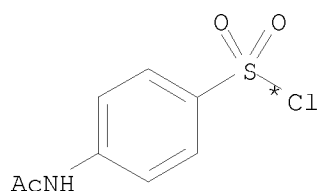
RX(52) OF 61 COMPOSED OF RX(2), RX(6), RX(12)  
 RX(52) F + G + S ==> Y



F



G

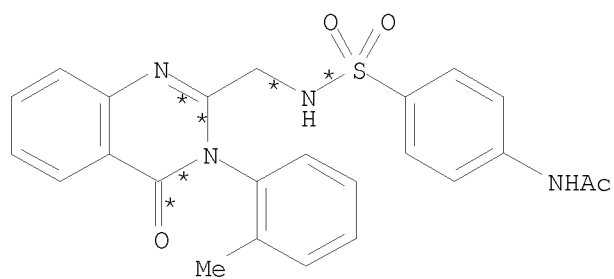


S

3  
 STEPS  
 →



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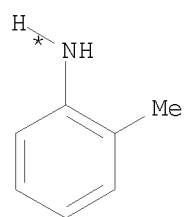
Y

RX(2) RCT F 95-53-4, G 14422-49-2  
 RGT D 7719-12-2 PC13  
 PRO H 3166-54-9  
 SOL 108-88-3 PhMe

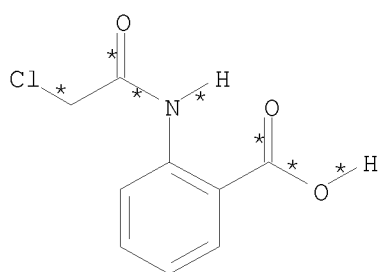
RX(6) RCT H 3166-54-9  
 RGT N 7664-41-7 NH3  
 PRO P 80096-33-9  
 SOL 110-86-1 Pyridine

RX(12) RCT S 121-60-8, P 80096-33-9  
 PRO Y 103953-06-6  
 SOL 110-86-1 Pyridine

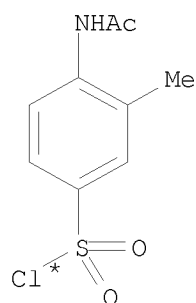
RX(53) OF 61 COMPOSED OF RX(2), RX(6), RX(13)  
 RX(53) F + G + Z ==> AA



F



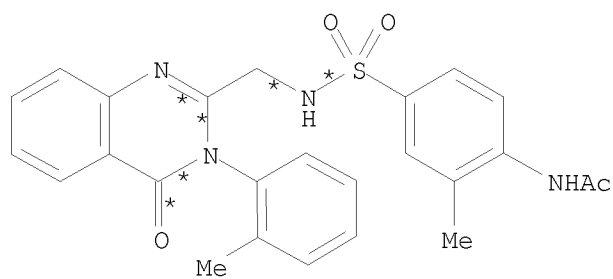
G



Z

3  
 STEPS  
 →

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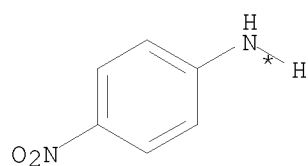
AA

RX(2) RCT F 95-53-4, G 14422-49-2  
RGT D 7719-12-2 PC13  
PRO H 3166-54-9  
SOL 108-88-3 PhMe

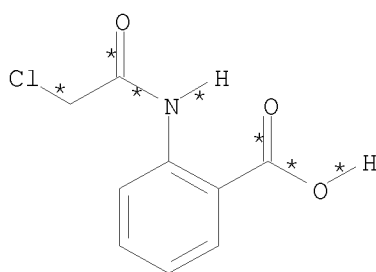
RX(6) RCT H 3166-54-9  
RGT N 7664-41-7 NH3  
PRO P 80096-33-9  
SOL 110-86-1 Pyridine

RX(13) RCT Z 14988-21-7, P 80096-33-9  
PRO AA 103953-07-7  
SOL 110-86-1 Pyridine

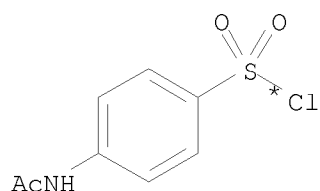
RX(54) OF 61 COMPOSED OF RX(3), RX(7), RX(14)  
RX(54) I + G + S ==> AB



I



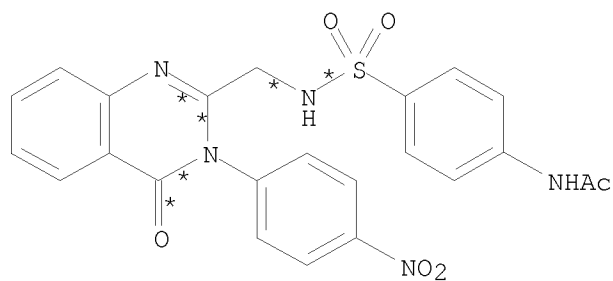
G



S

3  
STEPS  
→

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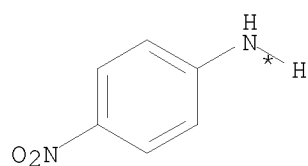
AB

RX(3) RCT I 100-01-6, G 14422-49-2  
RGT D 7719-12-2 PC13  
PRO J 103952-90-5  
SOL 108-88-3 PhMe

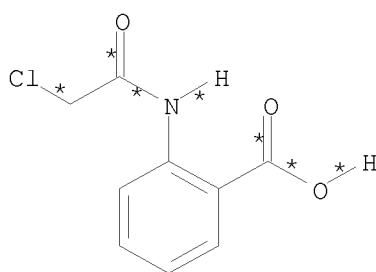
RX(7) RCT J 103952-90-5  
RGT N 7664-41-7 NH3  
PRO Q 103952-92-7  
SOL 110-86-1 Pyridine

RX(14) RCT S 121-60-8, Q 103952-92-7  
PRO AB 103953-00-0  
SOL 110-86-1 Pyridine

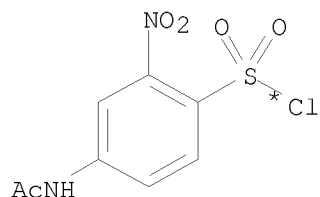
RX(55) OF 61 COMPOSED OF RX(3), RX(7), RX(15)  
RX(55) I + G + W ==> AC



I



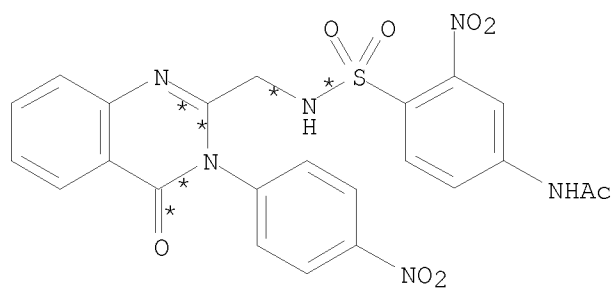
G



W

3  
STEPS  
→

10/ 562,112



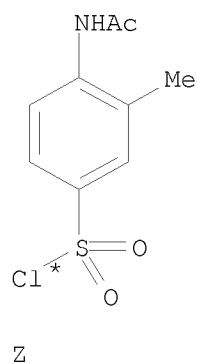
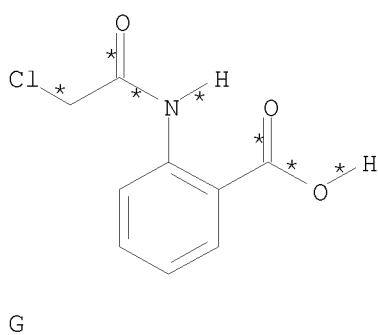
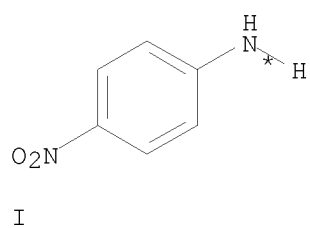
AC

RX(3)      RCT    I 100-01-6, G 14422-49-2  
             RGT    D 7719-12-2 PC13  
             PRO    J 103952-90-5  
             SOL    108-88-3 PhMe

RX(7)      RCT    J 103952-90-5  
             RGT    N 7664-41-7 NH3  
             PRO    Q 103952-92-7  
             SOL    110-86-1 Pyridine

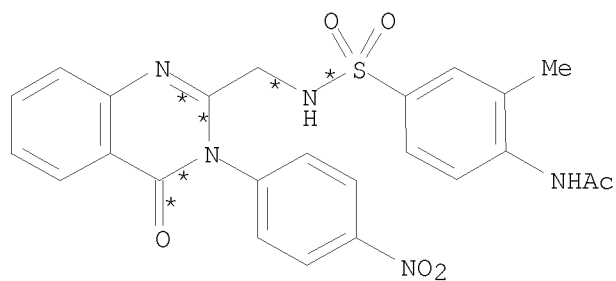
RX(15)     RCT    W 19300-50-6, Q 103952-92-7  
             PRO    AC 103953-01-1  
             SOL    110-86-1 Pyridine

RX(56) OF 61 COMPOSED OF RX(3), RX(7), RX(16)  
RX(56)      I    +    G    +    Z    ==>    AD



3  
STEPS  
→

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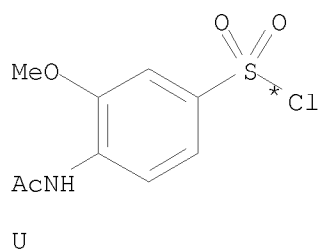
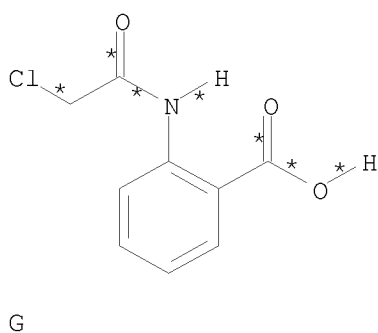
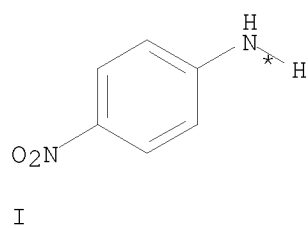
AD

RX(3) RCT I 100-01-6, G 14422-49-2  
RGT D 7719-12-2 PC13  
PRO J 103952-90-5  
SOL 108-88-3 PhMe

RX(7) RCT J 103952-90-5  
RGT N 7664-41-7 NH3  
PRO Q 103952-92-7  
SOL 110-86-1 Pyridine

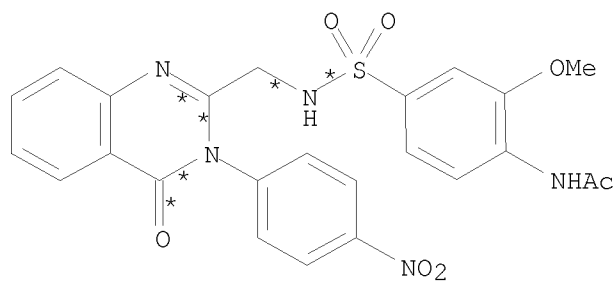
RX(16) RCT Z 14988-21-7, Q 103952-92-7  
PRO AD 103953-02-2  
SOL 110-86-1 Pyridine

RX(57) OF 61 COMPOSED OF RX(3), RX(7), RX(17)  
RX(57) I + G + U ==> AE



3  
STEPS  
→

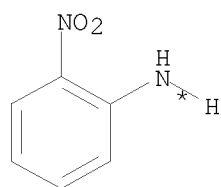
10/ 562,112



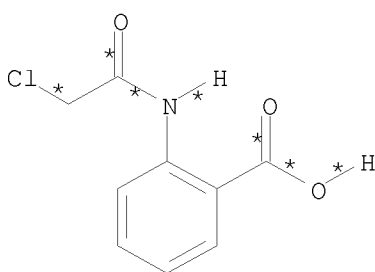
AE

RX(3)	RCT	I 100-01-6, G 14422-49-2
	RGT	D 7719-12-2 PC13
	PRO	J 103952-90-5
	SOL	108-88-3 PhMe
 RX(7)	RCT	J 103952-90-5
	RGT	N 7664-41-7 NH3
	PRO	Q 103952-92-7
	SOL	110-86-1 Pyridine
 RX(17)	RCT	U 46713-94-4, Q 103952-92-7
	PRO	AE 103953-03-3
	SOL	110-86-1 Pyridine

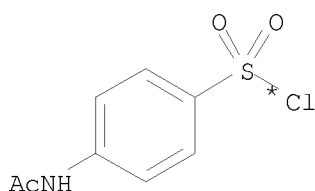
RX(58) OF 61 COMPOSED OF RX(4), RX(8), RX(18)  
 RX(58) K + G + S ==> AF



K



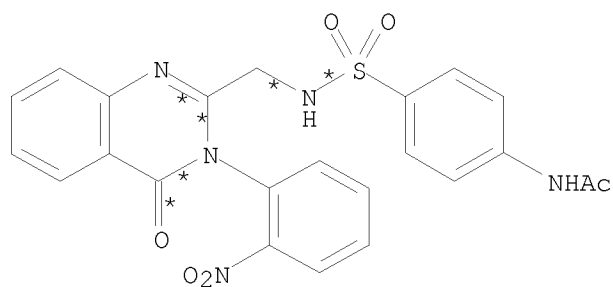
G



S

3  
 STEPS  
 →

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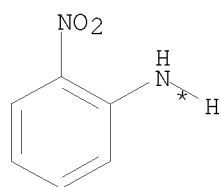
AF

RX(4) RCT K 88-74-4, G 14422-49-2  
 RGT D 7719-12-2 PC13  
 PRO L 80096-22-6  
 SOL 108-88-3 PhMe

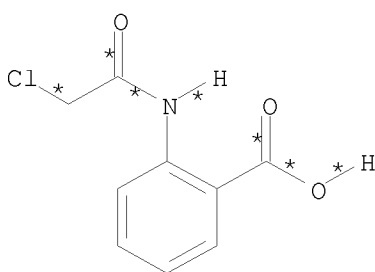
RX(8) RCT L 80096-22-6  
 RGT N 7664-41-7 NH3  
 PRO R 103952-93-8  
 SOL 110-86-1 Pyridine

RX(18) RCT S 121-60-8, R 103952-93-8  
 PRO AF 103953-08-8  
 SOL 110-86-1 Pyridine

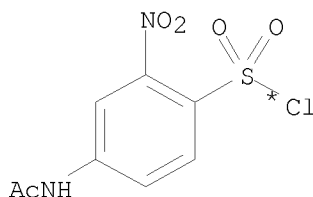
RX(59) OF 61 COMPOSED OF RX(4), RX(8), RX(19)  
 RX(59) K + G + W ==> AG



K



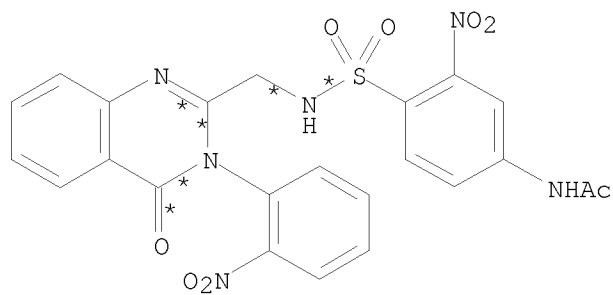
G



W

3  
 STEPS  
 →

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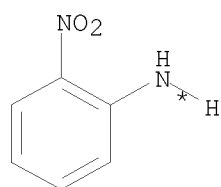
AG

RX(4) RCT K 88-74-4, G 14422-49-2  
 RGT D 7719-12-2 PC13  
 PRO L 80096-22-6  
 SOL 108-88-3 PhMe

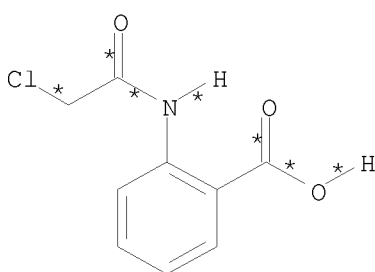
RX(8) RCT L 80096-22-6  
 RGT N 7664-41-7 NH3  
 PRO R 103952-93-8  
 SOL 110-86-1 Pyridine

RX(19) RCT W 19300-50-6, R 103952-93-8  
 PRO AG 103953-09-9  
 SOL 110-86-1 Pyridine

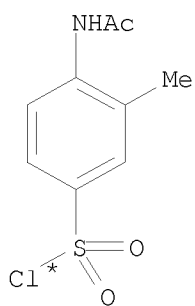
RX(60) OF 61 COMPOSED OF RX(4), RX(8), RX(20)  
 RX(60) K + G + Z ==> AH



K



G

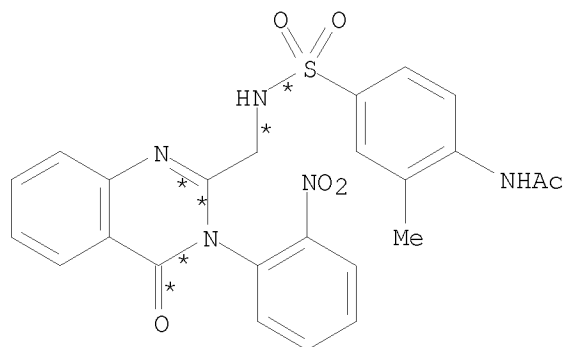


Z

3  
 STEPS  
 →



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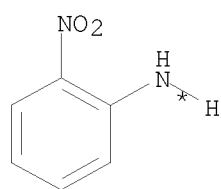
AH

RX(4) RCT K 88-74-4, G 14422-49-2  
RGT D 7719-12-2 PC13  
PRO L 80096-22-6  
SOL 108-88-3 PhMe

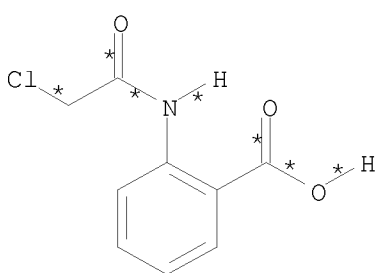
RX(8) RCT L 80096-22-6  
RGT N 7664-41-7 NH3  
PRO R 103952-93-8  
SOL 110-86-1 Pyridine

RX(20) RCT Z 14988-21-7, R 103952-93-8  
PRO AH 103953-10-2  
SOL 110-86-1 Pyridine

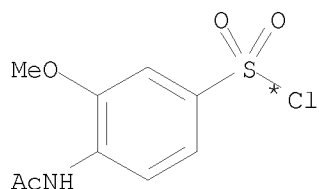
RX(61) OF 61 COMPOSED OF RX(4), RX(8), RX(21)  
RX(61) K + G + U ==> AI



K

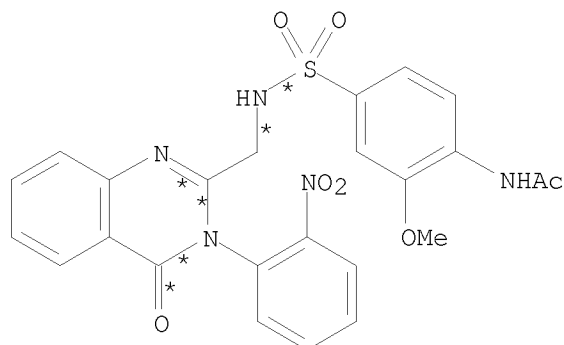


G



U

3  
STEPS  
=>



AI

RX(4) RCT K 88-74-4, G 14422-49-2  
 RGT D 7719-12-2 PC13  
 PRO L 80096-22-6  
 SOL 108-88-3 PhMe

RX(8) RCT L 80096-22-6  
 RGT N 7664-41-7 NH3  
 PRO R 103952-93-8  
 SOL 110-86-1 Pyridine

RX(21) RCT U 46713-94-4, R 103952-93-8  
 PRO AI 103953-11-3  
 SOL 110-86-1 Pyridine

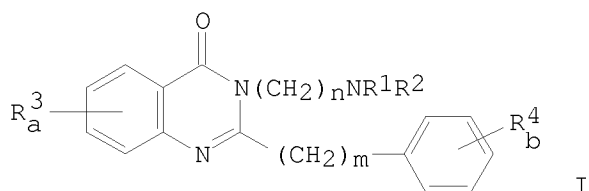
L3 ANSWER 195 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 105:60629 CASREACT  
 TITLE: 2-Phenylalkyl-3-aminoalkyl-4(3H)-quinazolinones,  
 pharmaceutical compositions and use  
 INVENTOR(S): Sekiya, Tetsuo; Tsutsui, Mikio; Horii, Daijiro;  
 Ishibashi, Akira  
 PATENT ASSIGNEE(S): Mitsubishi Yuka Pharmaceutical Co., Ltd., Japan  
 SOURCE: Eur. Pat. Appl., 58 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 169537	A2	19860129	EP 1985-109193	19850723
EP 169537	A3	19870325		
EP 169537	B1	19900103		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
JP 61036273	A	19860220	JP 1984-154086	19840726
US 4668682	A	19870526	US 1985-753708	19850710
CA 1266266	A1	19900227	CA 1985-486793	19850715
AT 49199	T	19900115	AT 1985-109193	19850723

DK 8503396	A	19860127	DK 1985-3396	19850725
HU 39166	A2	19860828	HU 1985-2850	19850726
HU 194836	B	19880328		

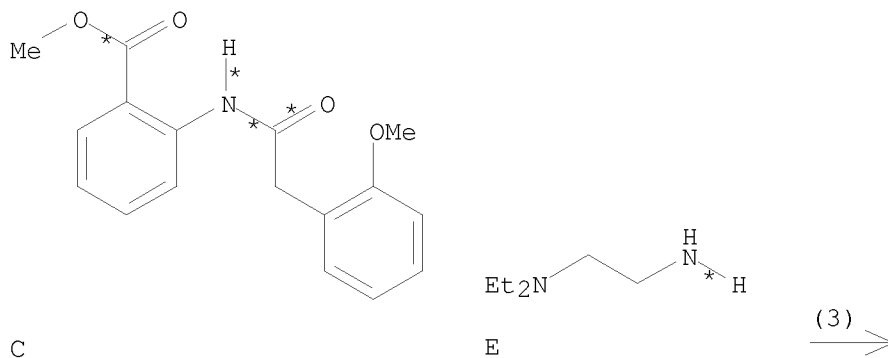
PRIORITY APPLN. INFO.: JP 1984-154086 19840726  
EP 1985-109193 19850723

OTHER SOURCE(S): MARPAT 105:60629  
GI

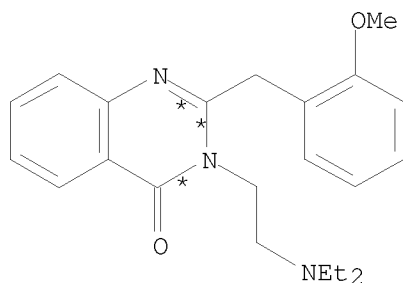


AB The title compds. I (R1 = H, C1-5 alkyl; R2 = C1-5 alkyl, (substituted) aralkyl; R3 = C1-5 alkyl or alkoxy, PhO, PhCH2O, HO, halogen; R4 = C1-5 alkyl or alkoxy, PhCH2O, NO2, halogen; R1NR2 may form a ring; a = 0-3; b = 1-3; m, n = 1-5) and their salts are Ca<sup>2+</sup> antagonists, vasodilators, and antagonists, vasodilators, and antihypertensives. For example, I (R1 = Me; R2 = 3,4-dimethoxyphenylethyl; R3 = 6-isopropoxy; R4 = 2,5-dimethoxy; m = 1; n = 2) (II) at  $\geq 0.03 \mu\text{M}$  inhibited the contraction of rat aortic strips induced by 10 mM Ca<sup>2+</sup> in the presence of 80 mM K<sup>+</sup>. II at 0.1 mg/kg i.v. increased the rate of coronary blood flow in dogs by 53.6%. II was prepared by condensation of the corresponding 2,6-disubstituted 4H-3,1-benzoxazin-4-one with 2-[N-(3,4-dimethoxyphenylethyl)-N-methylamino]ethylamine.

RX(3) OF 6 ...C + E ==> F



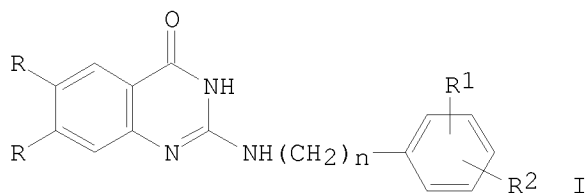
10/ 562,112



F

RX(3) RCT C 75256-36-9, E 100-36-7  
PRO F 103316-51-4

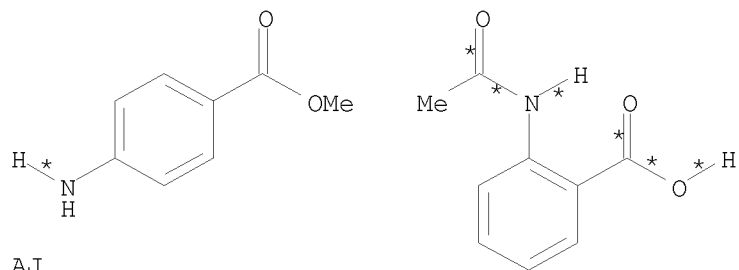
L3 ANSWER 196 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 104:186373 CASREACT  
TITLE: Design and synthesis of  
2-(arylamino)-4(3H)-quinazolinones as novel inhibitors  
of rat lens aldose reductase  
AUTHOR(S): DeRuiter, Jack; Brubaker, Abram N.; Millen, Jane;  
Riley, Thomas N.  
CORPORATE SOURCE: Sch. Pharm., Auburn Univ., Auburn, AL, 36849, USA  
SOURCE: Journal of Medicinal Chemistry (1986), 29(5), 627-9  
CODEN: JMCMAR; ISSN: 0022-2623  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Title quinazolinones I (R = H, MeO; R1 = H, 4-HO, 4-CO2H, 4-SO3Na, R2 = H; R1 = 3-HO, R2 = CO2H; n = 0, 1) which possess several of the pharmacophore moieties necessary for binding to the inhibitor site of aldose reductase, were prepared and tested for their ability to inhibit crude aldose reductase obtained from rat lens. Only those quinazolinones that possess an acidic moiety on the (arylamino) substituent were found to display significant inhibitory activity. The most potent compound is I (R = MeO, R1 = 4-CO2H, R2 = H, n = 0) with an IC50 of 34  $\mu$ M, while the least potent is I (R = H, R1 = 4-HO, R2 = H, n = 0) with an IC50 of 75  $\mu$ M.

RX(16) OF 49 AJ + AK ==> AL...

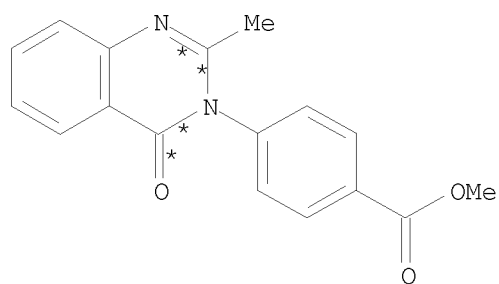
10/ 562,112



AJ

AK

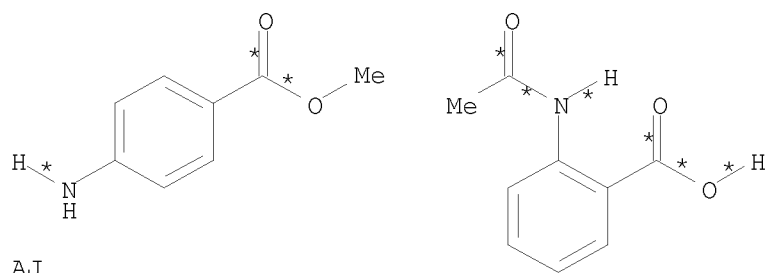
(16)  $\longrightarrow$



AL

RX(16)     RCT    AJ 619-45-4, AK 89-52-1  
               RGT    AM 7719-12-2 PC13  
               PRO    AL 35218-84-9  
               SOL    108-88-3 PhMe

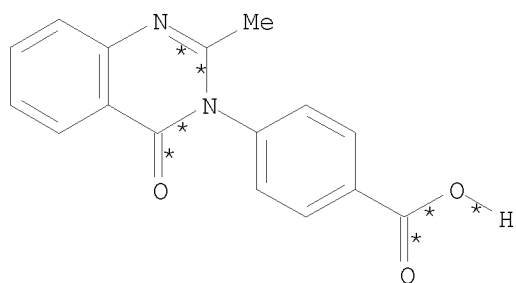
RX(31) OF 49 COMPOSED OF RX(16), RX(17)  
 RX(31)     AJ + AK ==> AO



AJ

AK

2  
 STEPS  
 $\longrightarrow$



AO

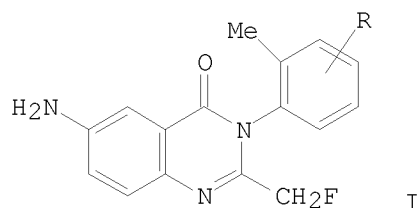
RX(16) RCT AJ 619-45-4, AK 89-52-1  
 RGT AM 7719-12-2 PC13  
 PRO AL 35218-84-9  
 SOL 108-88-3 PhMe

RX(17) RCT AL 35218-84-9  
 RGT X 7647-01-0 HCl  
 PRO AO 4005-05-4  
 SOL 7732-18-5 Water

L3 ANSWER 197 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 104:109677 CASREACT  
 TITLE: Quinazolinones  
 INVENTOR(S): Inoe, Kazumi; Oine, Toyao; Yamada, Yoshihisa; Ishida, Ryuichi; Ochiai, Takashi  
 PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 60178817	A	19850912	JP 1984-33251	19840222

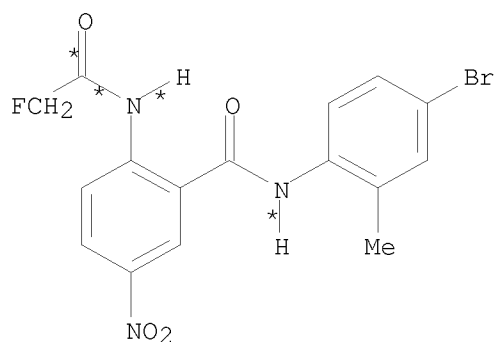
PRIORITY APPLN. INFO.: JP 1984-33251 19840222  
 GI



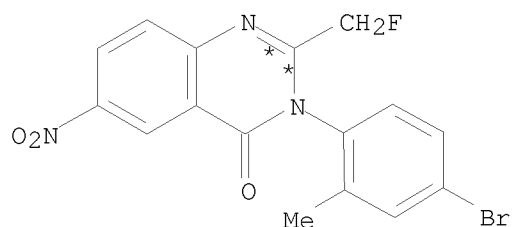
10/ 562,112

AB The title compds. (I; R = alkyl, alkoxy, halo), useful as muscle relaxants (no data), were prepared Thus, a mixture of 4.16 g 5-nitroisatoic anhydride, 3.6 g 2,4-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>NH<sub>2</sub>, and 25 mL xylene was refluxed for 30 min to give 82% 2,5-H<sub>2</sub>N(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>CONHC<sub>6</sub>H<sub>3</sub>Me<sub>2</sub>-2,4, which (4.0 g) in THF containing pyridine was treated with 2.18 g FCH<sub>2</sub>COCl at room temperature for 5 h to give 4.3 g 2,5-FCH<sub>2</sub>CONH(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>CONHC<sub>6</sub>H<sub>3</sub>Me<sub>2</sub>-2,4, which (4.0 g) was heated with BF<sub>3</sub>·Et<sub>2</sub>O in HOAc at 100-105° for 30 min to give 2.6 g 2-(fluoromethyl)-3-(2,4-dimethylphenyl)-4-nitro-4(3H)-quinazolinone, reduction of which (2.0 g) with SnCl<sub>2</sub> gave 1.2 g I (R = 4-Me).

RX(2) OF 12 ...B ==> C...



B

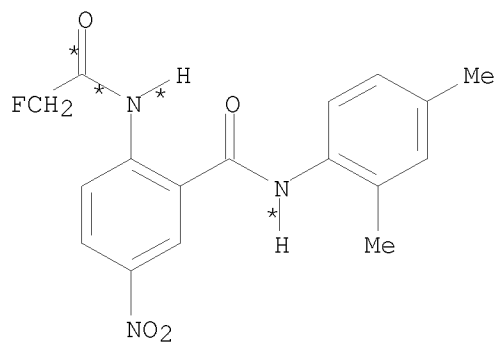


C

RX(2) RCT B 73832-54-9  
PRO C 73832-62-9

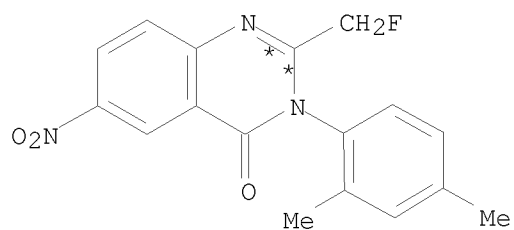
RX(5) OF 12 ...F ==> G...

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F

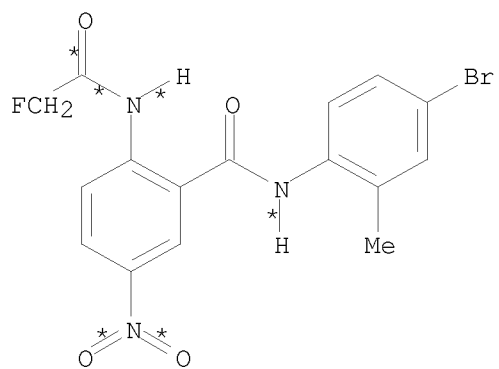
(5)  $\longrightarrow$



G

RX(5)      RCT   F 93670-44-1  
              PRO   G 93670-45-2

RX(8) OF 12 COMPOSED OF RX(2), RX(3)  
 RX(8)      B    ==>   D

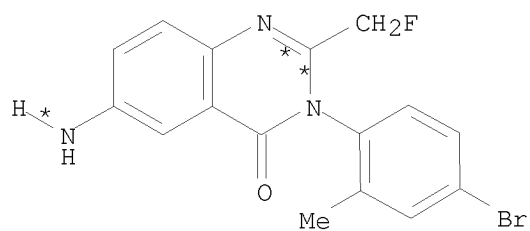


B

2  
 STEPS  
 $\longrightarrow$



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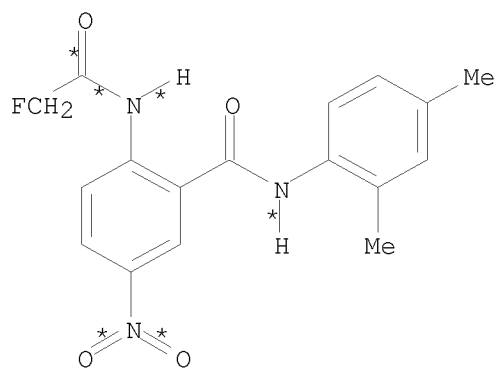


D

RX(2) RCT B 73832-54-9  
PRO C 73832-62-9

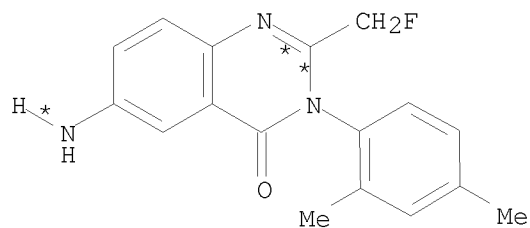
RX(3) RCT C 73832-62-9  
PRO D 73832-11-8

RX(10) OF 12 COMPOSED OF RX(5), RX(6)  
RX(10) F ==> H



F

2  
STEPS  
→



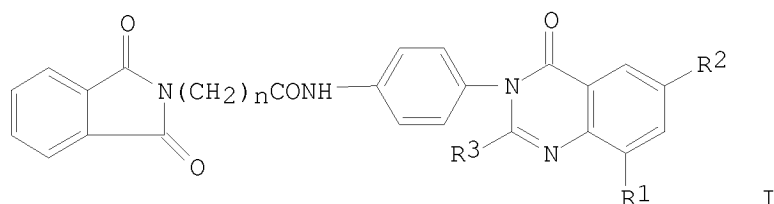
H

RX(5) RCT F 93670-44-1  
PRO G 93670-45-2

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RX(6) RCT G 93670-45-2  
PRO H 93670-47-4

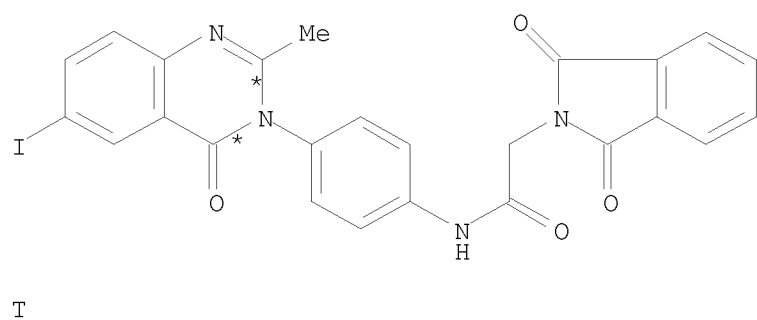
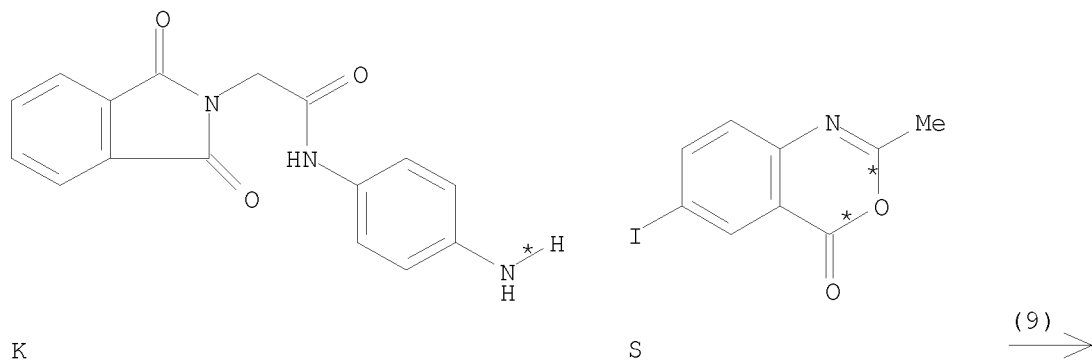
L3 ANSWER 198 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 104:81557 CASREACT  
TITLE: Synthesis of 6,8-disubstituted  
2-methyl/phenyl-3-[4-(3-phthalimido  
acetamido/propionamido)]phenylquinazolin-4-ones as  
anthelmintic agents  
AUTHOR(S): Shukla, J. S.; Srivastava, Beena  
CORPORATE SOURCE: Dep. Chem., Lucknow Univ., Lucknow, 226 001, India  
SOURCE: Current Science (1985), 54(22), 1162-4  
CODEN: CUSCAM; ISSN: 0011-3891  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Twelve title compds. (I; R1 = H or Br; R2 = H, Br, or I; R3 = Me or Ph; and n = 1 or 2) were prepared, by reaction of 2-(p-aminophenylacetamido)phthalamide [100278-18-0] or its propionamido homolog [100278-21-5] with 6,8-disubstituted 2-phenylbenzoxazin-4-ones, and screened for anthelmintic activity in mice, rats, and hamsters. All I were inactive as cestodicidal agents. I(R1 = R2 = Br and R3 = Ph) [100278-22-6] was the most active agent against *N. brasiliensis* infestation in rats; I(R1 = R2 = H and R3 = Me) [100278-15-7] was most active against *A. ceylanicum* infestation in hamsters. Some structure-activity relations are discussed briefly.

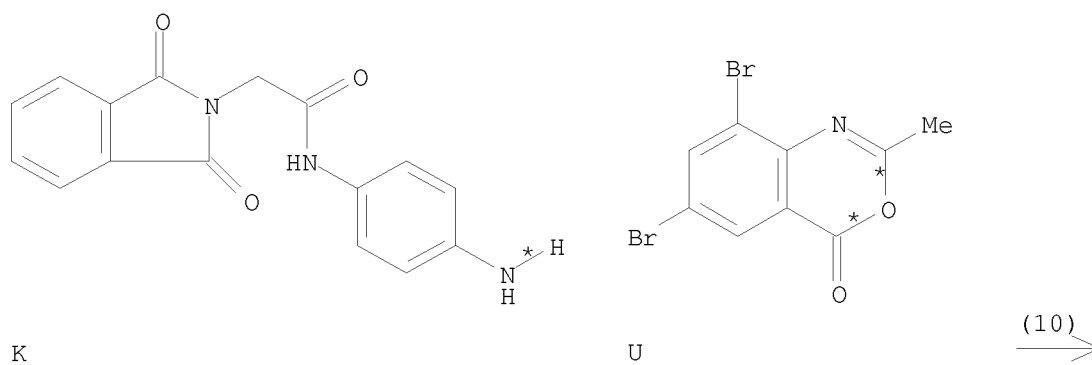
RX(9) OF 39 K + S ==> T

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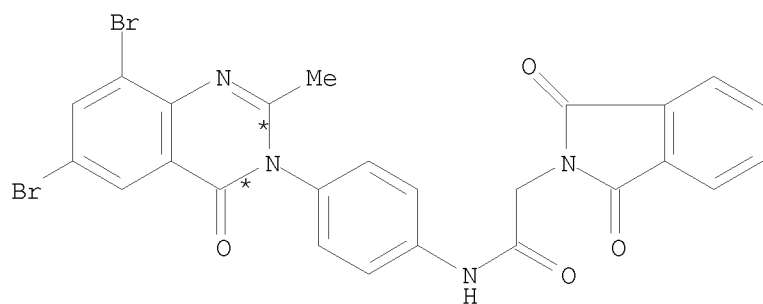


RX(9) RCT K 100278-18-0, S 40889-40-5  
 PRO T 100278-10-2  
 CAT 110-86-1 Pyridine

RX(10) OF 39 K + U  $\implies$  V



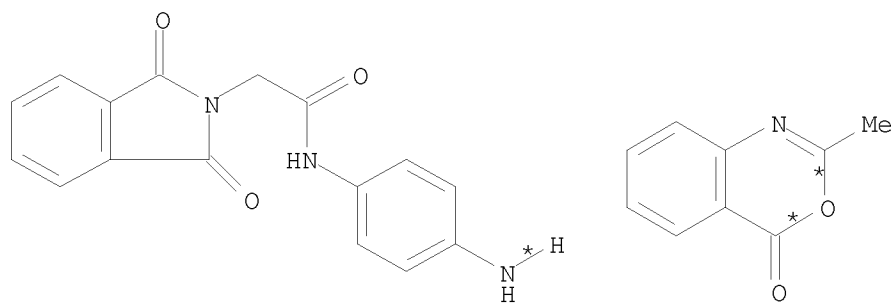
10/ 562,112



V

RX(10) RCT K 100278-18-0, U 40889-42-7  
 PRO V 100278-11-3  
 CAT 110-86-1 Pyridine

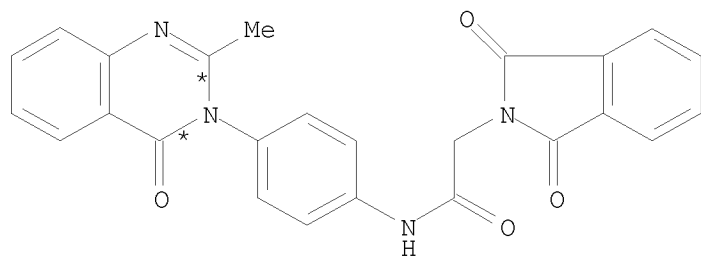
RX(11) OF 39 K + W ==> X



K

W

(11)  
 →

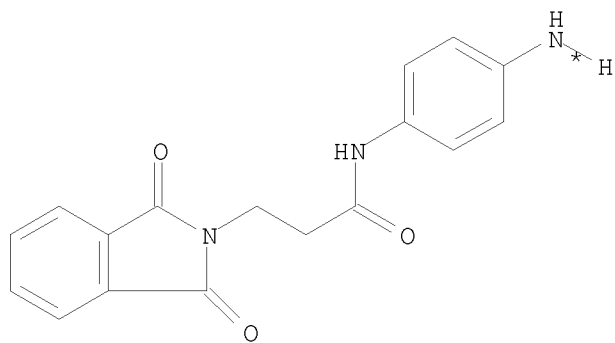


X

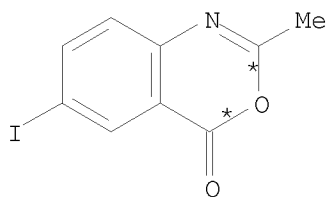
RX(11) RCT K 100278-18-0, W 525-76-8  
 PRO X 100278-12-4  
 CAT 110-86-1 Pyridine

10/ 562,112

RX(15) OF 39      ...I + S ==> AB

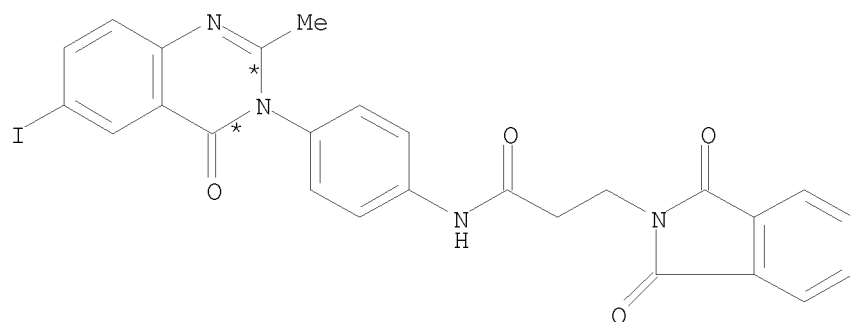


I



S

(15)  
→

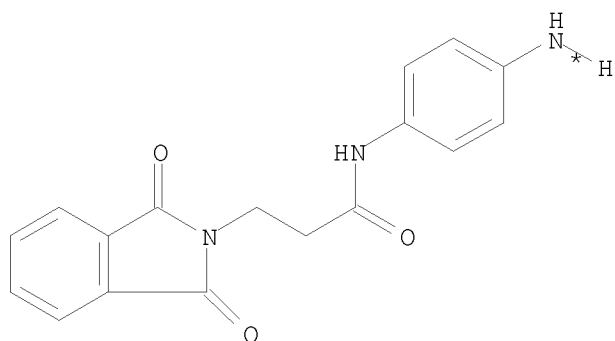


AB

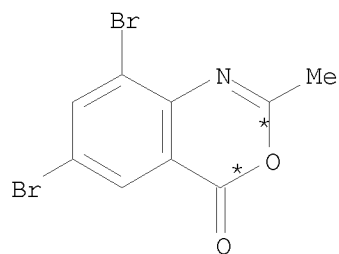
RX(15)      RCT    I 100278-21-5, S 40889-40-5  
              PRO    AB 100828-89-5  
              CAT    110-86-1 Pyridine

RX(16) OF 39      ...I + U ==> AC

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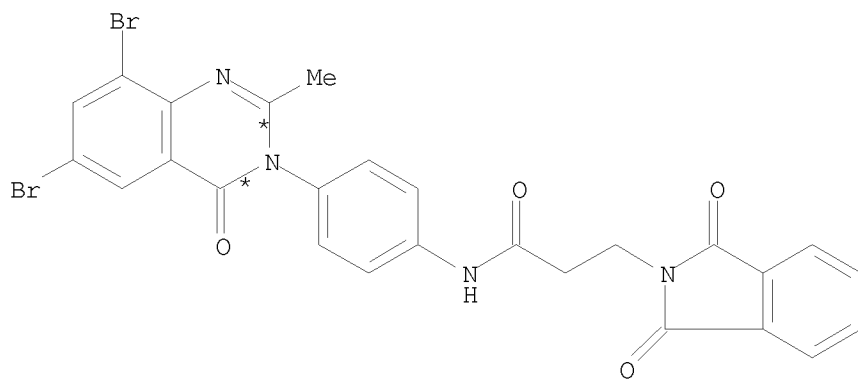


I



U

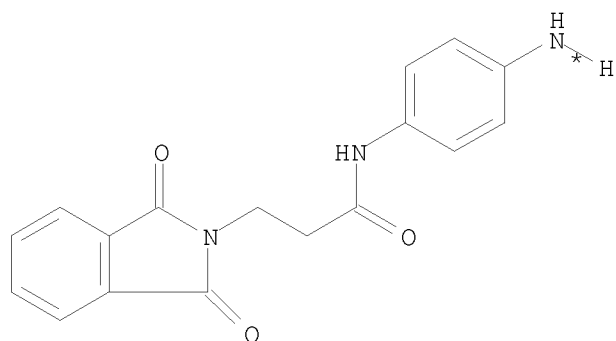
(16)  
→



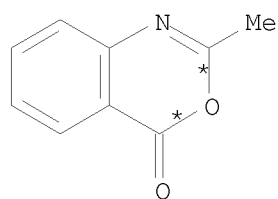
AC

RX(16)     RCT   I 100278-21-5, U 40889-42-7  
             PRO   AC 100278-16-8  
             CAT   110-86-1 Pyridine

RX(17) OF 39     ...I   +   W   ==>   AD

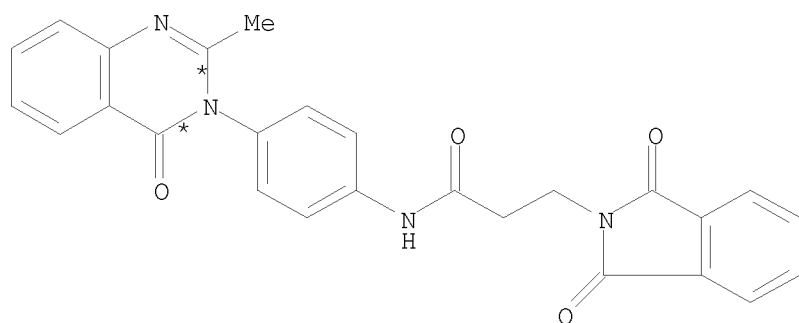


I



W

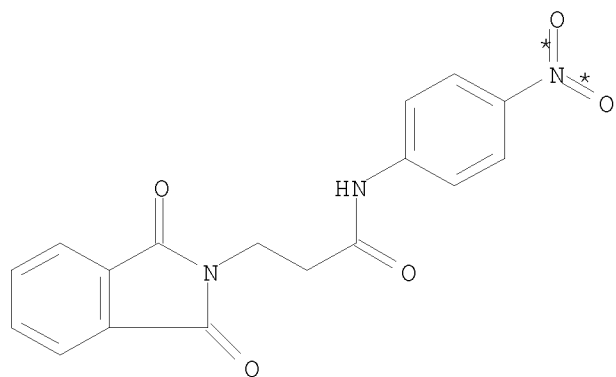
(17)  $\longrightarrow$



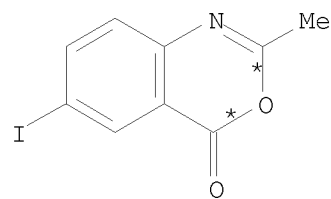
AD

RX(17) RCT I 100278-21-5, W 525-76-8  
 PRO AD 100278-15-7  
 CAT 110-86-1 Pyridine

RX(24) OF 39 COMPOSED OF RX(5), RX(15)  
 RX(24) H + S ==> AB



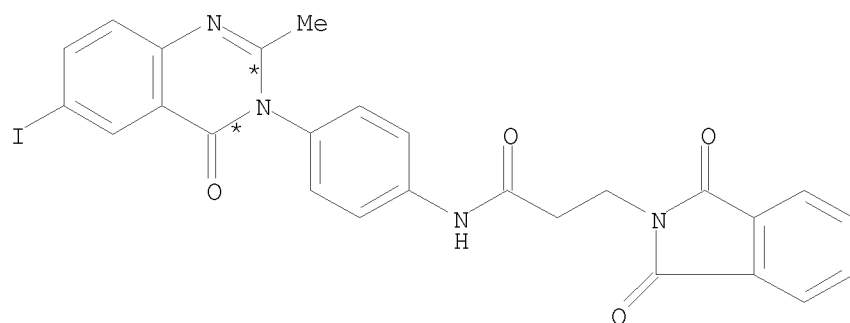
H



S

10/ 562,112

2  
STEPS  
→

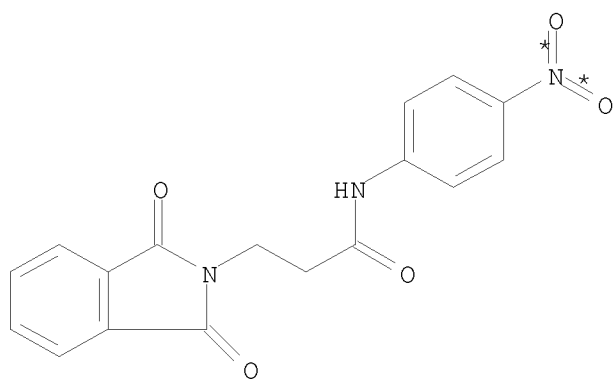


AB

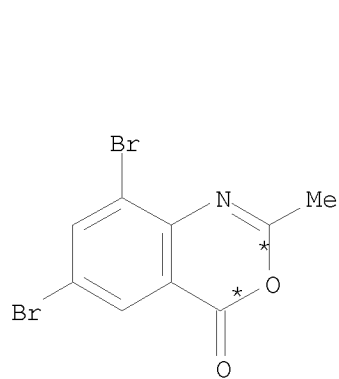
RX(5) RCT H 100278-17-9  
RGT J 302-01-2 N2H4  
PRO I 100278-21-5

RX(15) RCT I 100278-21-5, S 40889-40-5  
PRO AB 100828-89-5  
CAT 110-86-1 Pyridine

RX(25) OF 39 COMPOSED OF RX(5), RX(16)  
RX(25) H + U ==> AC



H

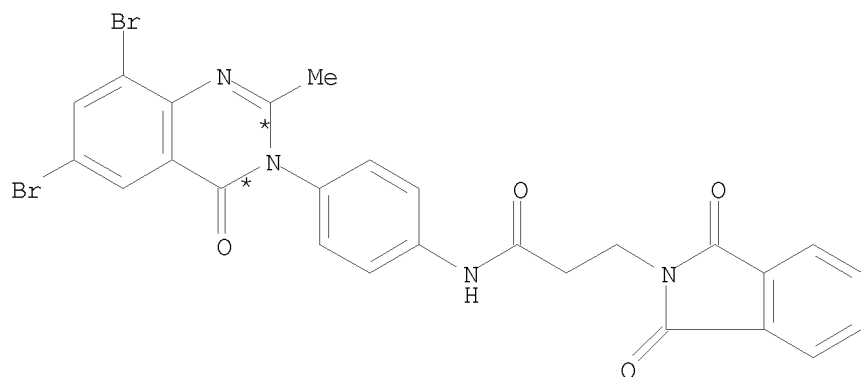


U

2  
STEPS  
→



10/ 562,112

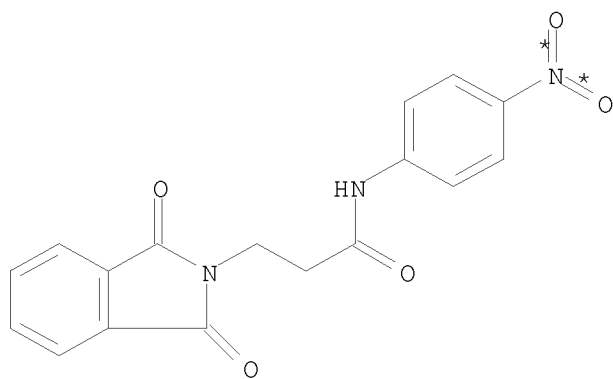


AC

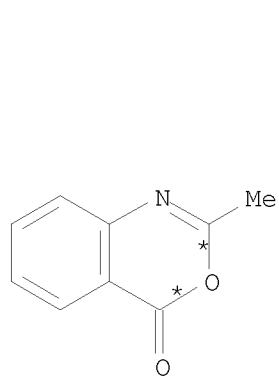
RX(5) RCT H 100278-17-9  
RGT J 302-01-2 N2H4  
PRO I 100278-21-5

RX(16) RCT I 100278-21-5, U 40889-42-7  
PRO AC 100278-16-8  
CAT 110-86-1 Pyridine

RX(26) OF 39 COMPOSED OF RX(5), RX(17)  
RX(26) H + W ==> AD

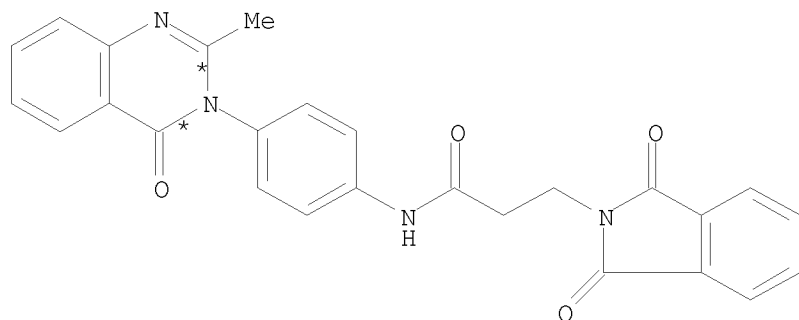


H



W

2  
STEPS  
→

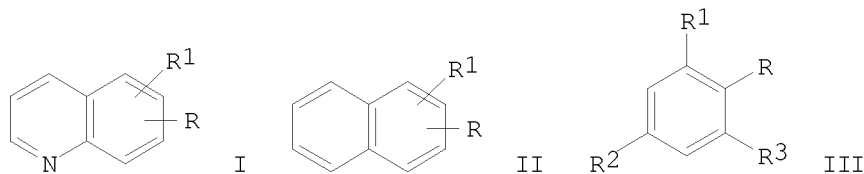


AD

RX(5) RCT H 100278-17-9  
 RGT J 302-01-2 N2H4  
 PRO I 100278-21-5

RX(17) RCT I 100278-21-5, W 525-76-8  
 PRO AD 100278-15-7  
 CAT 110-86-1 Pyridine

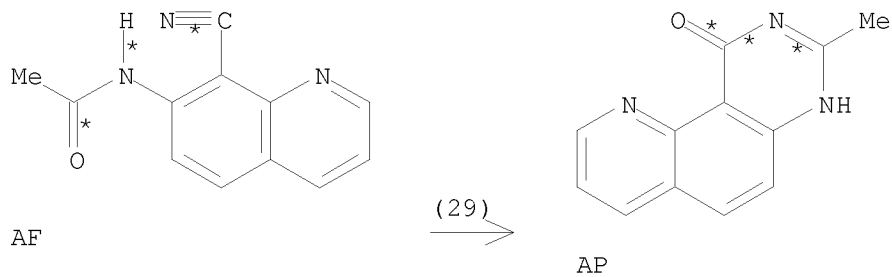
L3 ANSWER 199 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 103:104667 CASREACT  
 TITLE: Studies on aromatic nitro compounds. V. A simple one-pot preparation of o-aminoaroylnitriles from some aromatic nitro compounds  
 AUTHOR(S): Tomioka, Yukihiro; Ohkubo, Kimiko; Yamazaki, Motoyoshi  
 CORPORATE SOURCE: Fac. Pharm. Sci., Fukuoka Univ., Fukuoka, 814-01, Japan  
 SOURCE: Chemical & Pharmaceutical Bulletin (1985), 33(4), 1360-6  
 CODEN: CPBTAL; ISSN: 0009-2363  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB The reactions of aromatic nitro compds. I, II (R = H, R1 = NO2), and III (R, R1 = same, R2 = CF3, MeCO, PhCO, R3 = H ; R2 = R3 = CF3) with Et cyanoacetate and KOH in DMF followed by hydrolysis of the reaction mixture with HCl or NaOH gave the corresponding o-aminoaroylnitriles I-III (R = CN, R1 = NH2). Acetylation-cyclization reactions of the products were carried out.

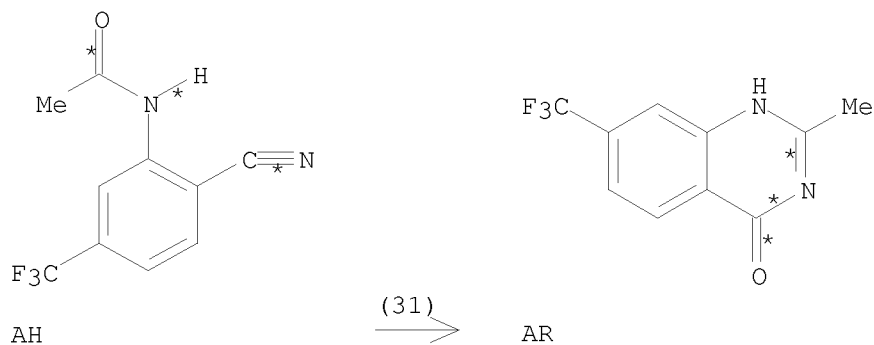
10/ 562,112

RX(29) OF 55 ...AF ==> AP



RX(29) RCT AF 98012-90-9  
RGT E 7647-01-0 HCl  
PRO AP 98012-97-6  
SOL 64-17-5 EtOH

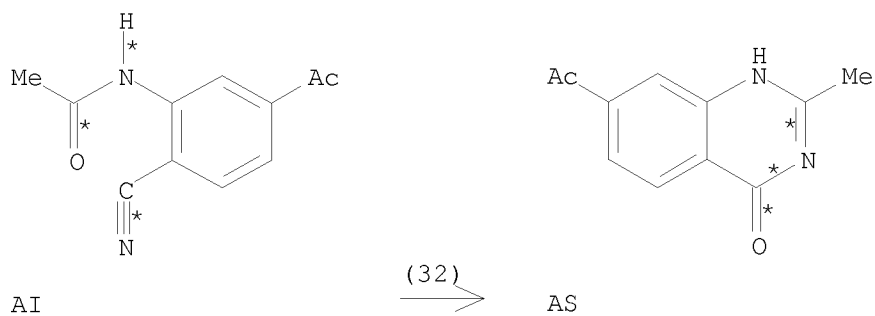
RX(31) OF 55 ...AH ==> AR



RX(31) RCT AH 98012-92-1  
RGT E 7647-01-0 HCl  
PRO AR 35241-26-0  
SOL 64-17-5 EtOH

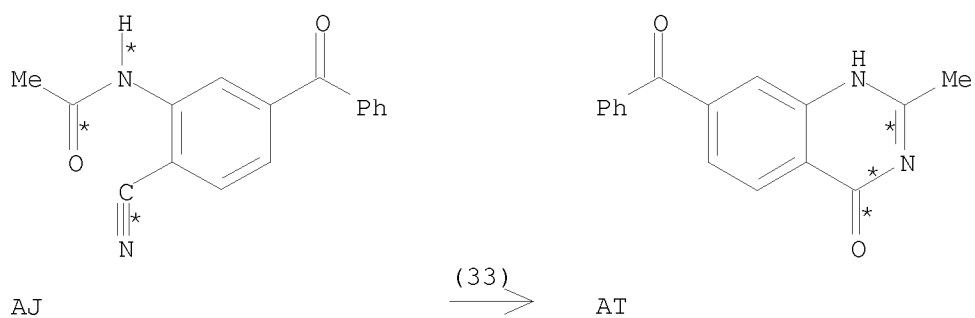
RX(32) OF 55 ...AI ==> AS

10/ 562,112



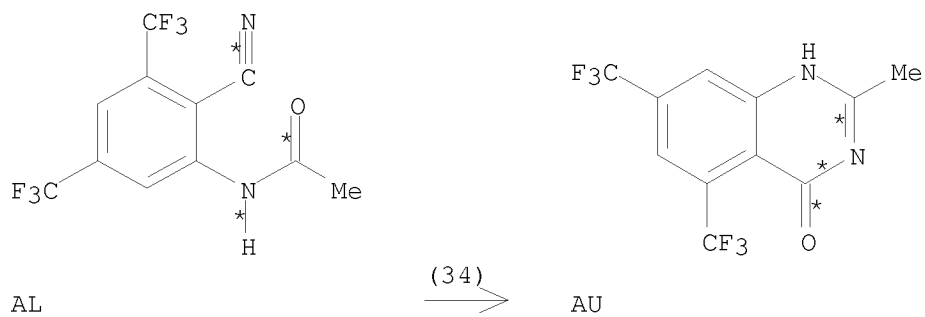
RX(32) RCT AI 98012-93-2  
RGT E 7647-01-0 HCl  
PRO AS 98012-99-8  
SOL 64-17-5 EtOH

RX(33) OF 55 ...AJ ==> AT



RX(33) RCT AJ 98012-94-3  
RGT E 7647-01-0 HCl  
PRO AT 98013-00-4  
SOL 64-17-5 EtOH

RX(34) OF 55 ...AL ==> AU



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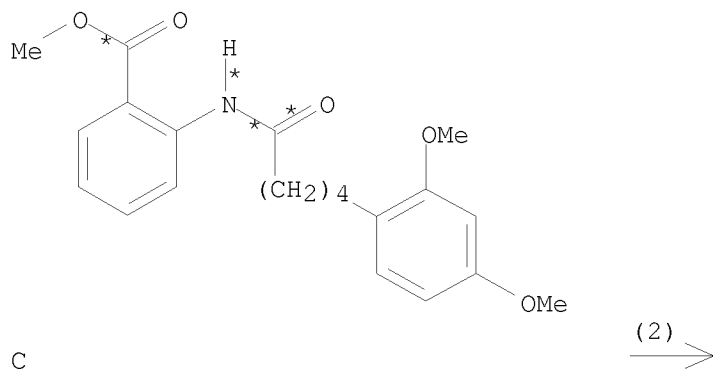
RX(34)     RCT    AL 98012-95-4  
           RGT    E 7647-01-0 HCl  
           PRO    AU 98013-01-5  
           SOL    64-17-5 EtOH

L3    ANSWER 200 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER:        103:54028    CASREACT  
TITLE:                    Intramolecular reactions of N-nitrenes: oxidation of  
                             3-amino-2-(2,4-dimethoxyphenylbutyl)quinazolin-4(3H)-  
                             ones  
AUTHOR(S):                Atkinson, Robert S.; Gawad, Nagwa A.  
CORPORATE SOURCE:        Dep. Chem., Univ. Leicester, Leicester, LE1 7RH, UK  
SOURCE:                    Journal of the Chemical Society, Perkin Transactions  
                             1: Organic and Bio-Organic Chemistry (1972-1999)  
                             (1985), (4), 825-30  
                             CODEN: JCPRB4; ISSN: 0300-922X  
DOCUMENT TYPE:            Journal  
LANGUAGE:                 English  
GI

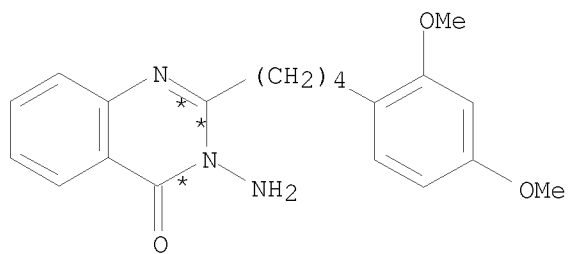
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB    The N-nitrenes generated by oxidation of the title compds. I (R = H, Me) were trapped by the remote 2,4-dimethoxyphenyl ring. Thus, oxidation of I (R = Me) by Pb(OAc)<sub>4</sub> in C<sub>6</sub>H<sub>6</sub> gave 60% metacyclophane II, whereas oxidation in MeOH gave III, IV, and V; the structures of III and V were confirmed by x-ray anal. Oxidation of I (R = H) in MeOH and in C<sub>6</sub>H<sub>6</sub> containing CH<sub>2</sub>:CHCH<sub>2</sub>OH gave VI and VII, resp. An explanation is given for the regiochem. of the trapping reaction.

RX(2) OF 35        ...C ==> E...



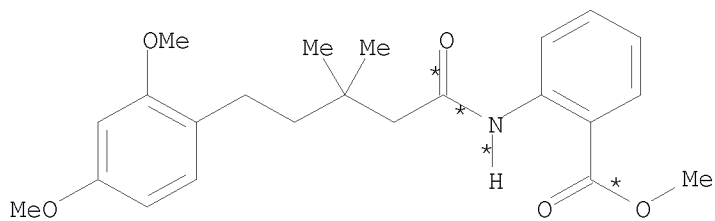
10/ 562,112



E

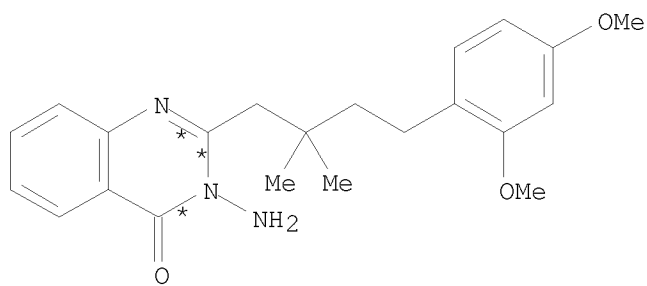
RX (2)	RCT	C 97305-81-2
	RGT	F 302-01-2 N2H4
	PRO	E 97305-82-3
	SOL	64-17-5 EtOH

RX(8) OF 35 . . . T ==> U . . .



T

(8) 



U

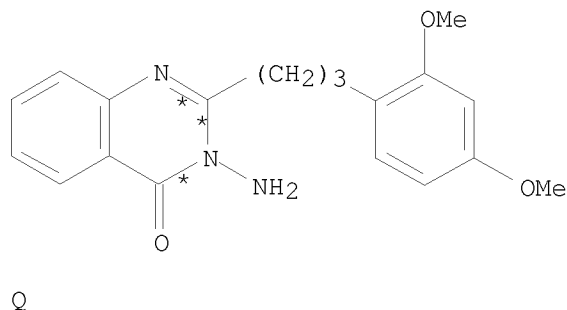
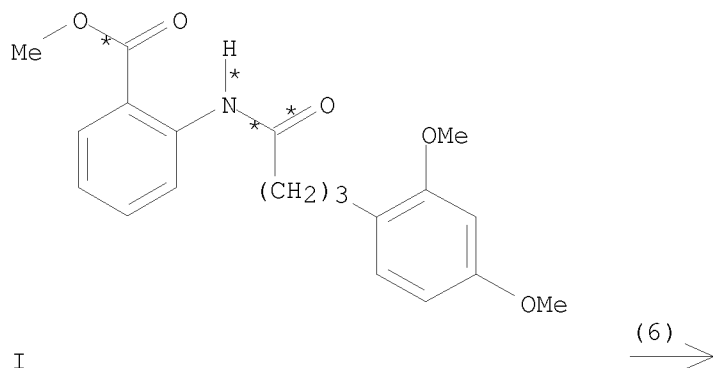
RX (8)	RCT	T 97305-85-6
	RGT	F 302-01-2 N2H4
	PRO	U 94922-06-2
	SOL	64-17-5 EtOH

L3 ANSWER 201 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 103:22566 CASREACT  
 TITLE: Intramolecular reactions of N-nitrenes: oxidation of  
 3-amino-2-(2,4-dimethoxyphenylpropyl)quinazolin-4(3H)-  
 one  
 AUTHOR(S): Atkinson, Robert S.; Gawad, Nagwa A.  
 CORPORATE SOURCE: Dep. Chem., Univ. Leicester, Leicester, LE1 7RH, UK  
 SOURCE: Journal of the Chemical Society, Perkin Transactions  
 1: Organic and Bio-Organic Chemistry (1972-1999)  
 (1985), (2), 341-4  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Oxidation of the title compound (I; R = H) or its di-Me analog I (R = Me) by Pb(OAc)<sub>4</sub> in MeOH containing K<sub>2</sub>CO<sub>3</sub> for 5 min gave the corresponding tetracycles II (R = H, Me) in 29 and 55% yield, resp. On standing overnight in MeOH, II (R = H) was converted quant. to the cyclopentane ring-containing analog III, the structure of which was determined by x-ray anal.

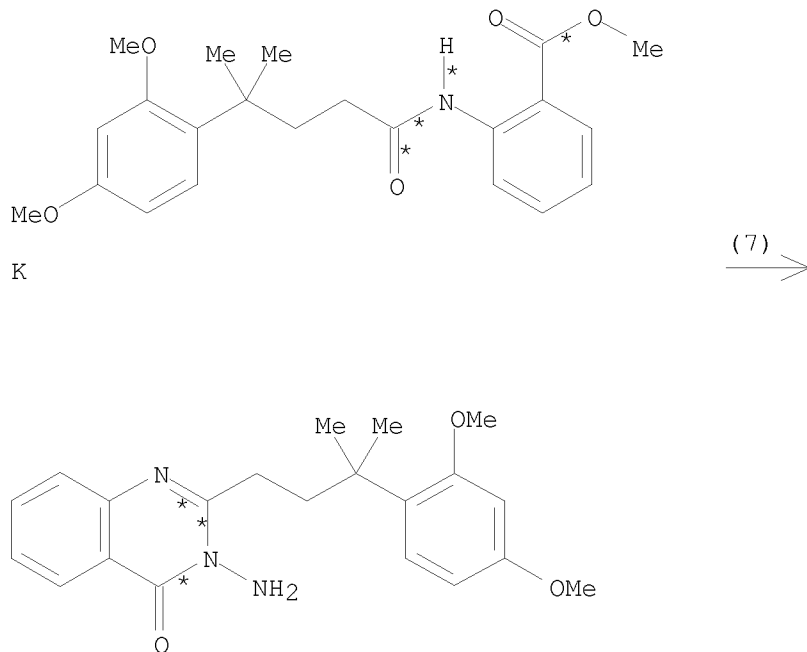
RX(6) OF 40 ...I ==> Q...



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RX(6) RCT I 96818-24-5  
RGT R 7803-57-8 N2H4-H2O  
PRO Q 87893-97-8  
SOL 64-17-5 EtOH

RX(7) OF 40 ...K ==> T...



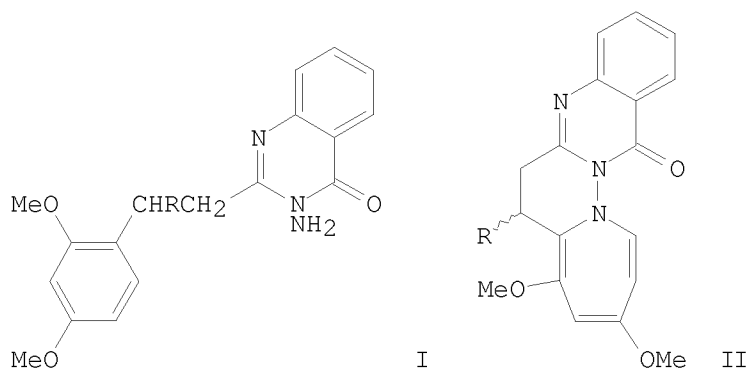
T

RX(7) RCT K 96818-25-6  
RGT R 7803-57-8 N2H4-H2O  
PRO T 87893-98-9  
SOL 64-17-5 EtOH

L3 ANSWER 202 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 103:22542 CASREACT  
TITLE: Intramolecular reactions of N-nitrenes: oxidation of  
3-amino-2-(2,4-dimethoxyphenylethyl)quinazolin-4(3H)-  
ones  
AUTHOR(S): Atkinson, Robert S.; Gawad, Nagwa A.  
CORPORATE SOURCE: Dep. Chem., Univ. Leicester, Leicester, LE1 7RH, UK  
SOURCE: Journal of the Chemical Society, Perkin Transactions  
1: Organic and Bio-Organic Chemistry (1972-1999)  
(1985), (2), 335-9  
CODEN: JCPRB4; ISSN: 0300-922X  
DOCUMENT TYPE: Journal  
LANGUAGE: English

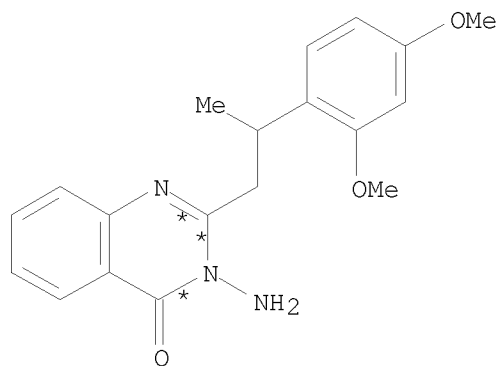
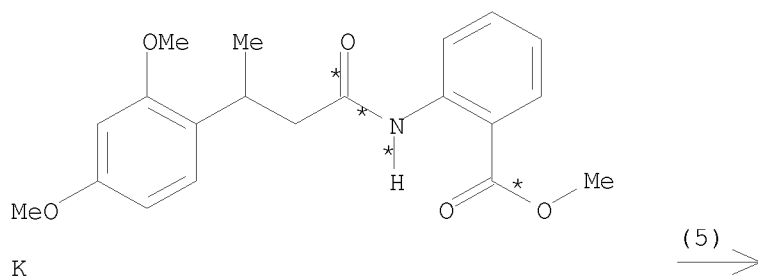


GI



AB Oxidation of the N-aminoquinazolones I ( $R = H, Me$ ) by  $Pb(OAc)_4$  in  $CHCl_3$  for 5 min gave the corresponding 1H-azepines II [ $R = H$  (III), endo-Me (IV)]. Boat-to-boat flipping of the azepine ring in III is slow on the NMR time-scale, even at  $140^\circ$ . Heating IV in  $PhCl$  at  $135^\circ$  gave the corresponding stereoisomer II ( $R = \text{exo-Me}$ ) with a min. free energy barrier of 30 kcal/mol. Reasons for the high barrier to azepine ring inversion are examined

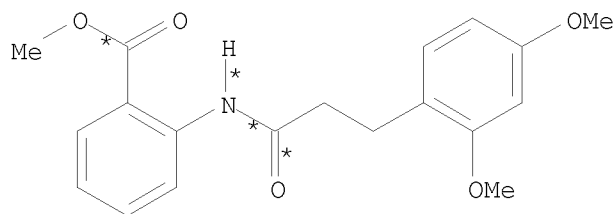
RX(5) OF 33      ...K ==> L...



10/ 562,112

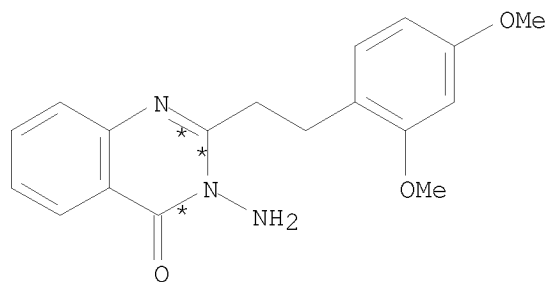
RX(5)        RCT    K 96818-14-3  
              RGT    M 7803-57-8 N2H4-H2O  
              PRO    L 92617-47-5  
              SOL    64-17-5 EtOH

RX(6) OF 33        ...I ==> O...



I

(6)  
→



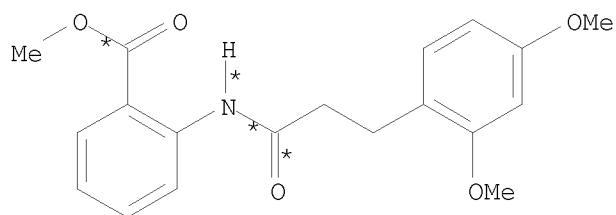
O

RX(6)        RCT    I 96818-15-4  
              RGT    M 7803-57-8 N2H4-H2O  
              PRO    O 92617-46-4  
              SOL    64-17-5 EtOH

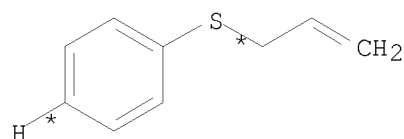
RX(19) OF 33 COMPOSED OF RX(6), RX(11)

RX(19)        I    +    Z    ==>    AA

10/ 562,112

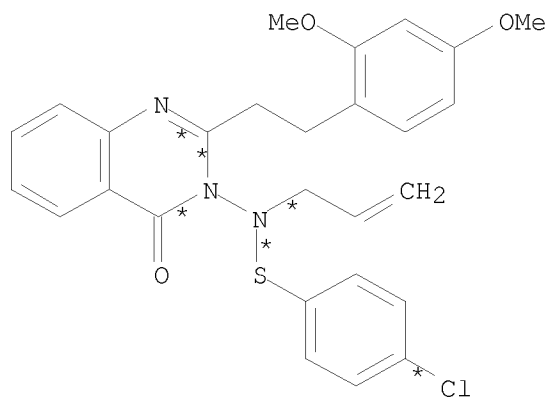


I



Z

2  
STEPS  
→

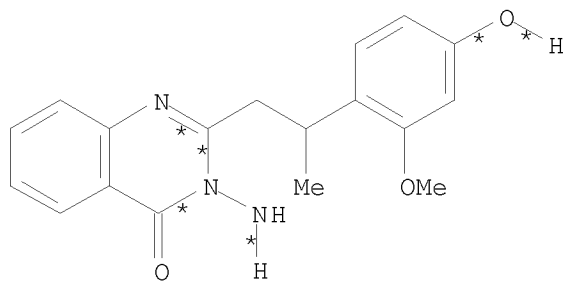
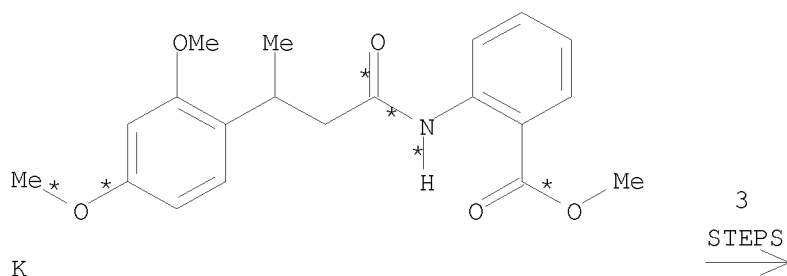


AA

RX(6)      RCT    I 96818-15-4  
             RGT    M 7803-57-8 N2H4-H2O  
             PRO    O 92617-46-4  
             SOL    64-17-5 EtOH

RX(11)     RCT    Z 5296-64-0, O 92617-46-4  
             RGT    Q 546-67-8 Pb(OAc)4  
             PRO    AA 92617-50-0  
             SOL    67-66-3 CHCl3

RX(31) OF 33 COMPOSED OF RX(5), RX(9), RX(10)  
RX(31)      K    ==>    V

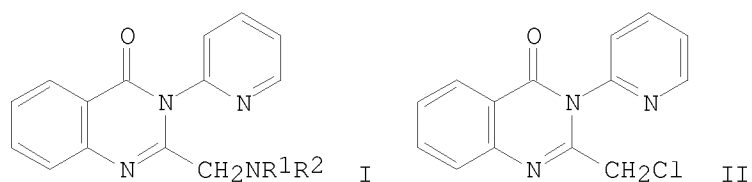


RX(5)	RCT	K 96818-14-3
	RGT	M 7803-57-8 N <sub>2</sub> H <sub>4</sub> -H <sub>2</sub> O
	PRO	L 92617-47-5
	SOL	64-17-5 EtOH
RX(9)	RCT	L 92617-47-5
	RGT	Q 546-67-8 Pb(OAc) <sub>4</sub>
	PRO	T 96818-16-5
	SOL	67-56-1 MeOH
RX(10)	RCT	T 96818-16-5
	RGT	W 7647-01-0 HCl, X 7440-66-6 Zn
	PRO	V 96818-17-6
	SOL	67-56-1 MeOH, 7732-18-5 Water

L3 ANSWER 203 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 102:220818 CASREACT  
 TITLE: Possible antifertility agents. Part-I. Synthesis of  
 2-(N,N-substituted-aminomethyl)-3-(2-pyridyl)-4(3H)-  
 oxo-3,1-quinazolines  
 AUTHOR(S): Kulkarni, Y. D.; Abdi, S. H. R.; Sharma, V. L.  
 CORPORATE SOURCE: Dep. Chem., Univ. Lucknow, Lucknow, 226 007, India  
 SOURCE: Journal of the Indian Chemical Society (1984), 61(8),  
 720-1  
 CODEN: JICSAH; ISSN: 0019-4522  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

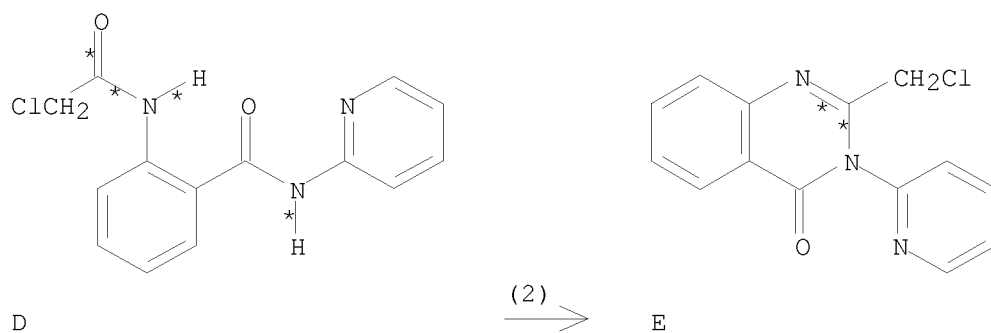
10/ 562,112

GI



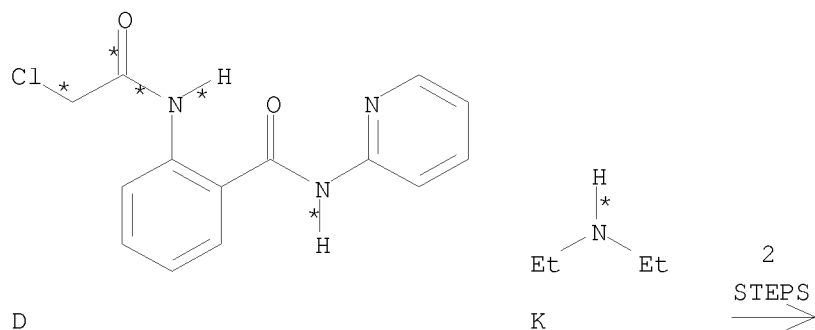
AB    The title compds. I (NR<sub>1</sub>R<sub>2</sub> = Et<sub>2</sub>N, pyrrolidino, piperidino, 4-methylpiperidino, morpholino), potential contraceptives, were prepared in 5 steps from o-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>COCl and 2-aminopyridine via o-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CONHR (R = 2-pyridyl), o-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CONHR, o-ClCH<sub>2</sub>CONHC<sub>6</sub>H<sub>4</sub>CONHR, and quinazolinone II. I showed little or no activity at 25 mg/kg animal (unidentified).

RX(2) OF 35            ...D ==> E...

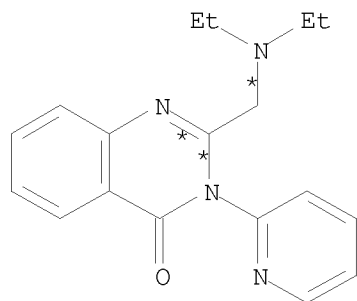


RX(2)            RCT   D 96656-50-7  
                   PRO   E 76535-05-2  
                   CAT   108-24-7 Ac2O

RX(11) OF 35 COMPOSED OF RX(2), RX(5)  
 RX(11)        D + K ==> L



10/ 562,112

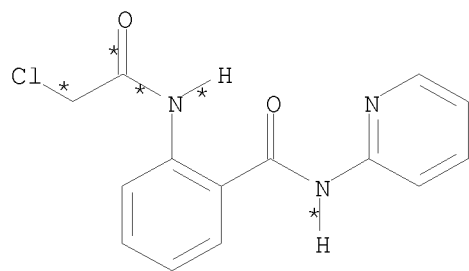


L

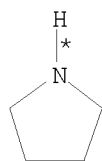
RX(2)      RCT   D 96656-50-7  
              PRO   E 76535-05-2  
              CAT   108-24-7 Ac2O

RX(5)      RCT   E 76535-05-2, K 109-89-7  
              PRO   L 96656-51-8  
              CAT   110-86-1 Pyridine

RX(12) OF 35 COMPOSED OF RX(2), RX(6)  
 RX(12)      D   +   N   ==>   O



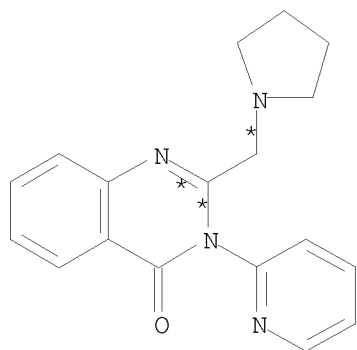
D



N

2  
 STEPS  
 →

10/ 562,112



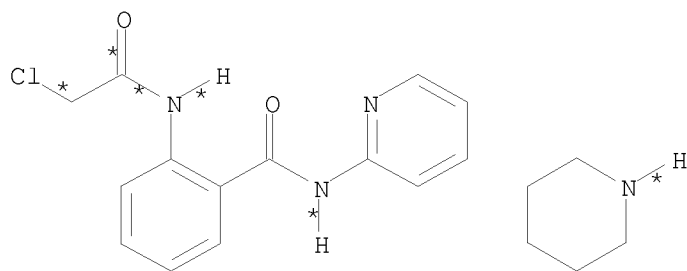
O

RX(2)        RCT   D 96656-50-7  
              PRO   E 76535-05-2  
              CAT   108-24-7 Ac2O

RX(6)        RCT   E 76535-05-2, N 123-75-1  
              PRO   O 96656-52-9

RX(13) OF 35 COMPOSED OF RX(2), RX(7)

RX(13)       D   +   P   ==>   Q

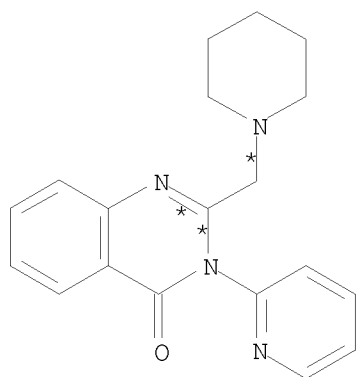


D

P

2  
STEPS  
→

10/ 562,112



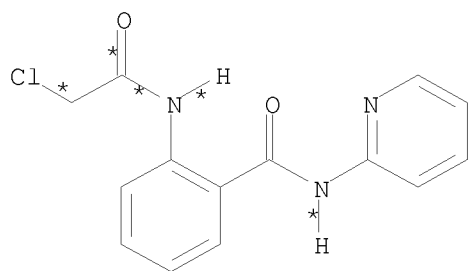
Q

RX(2)        RCT   D 96656-50-7  
              PRO   E 76535-05-2  
              CAT   108-24-7 Ac2O

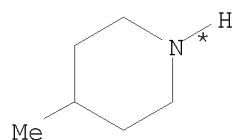
RX(7)        RCT   E 76535-05-2, P 110-89-4  
              PRO   Q 96656-53-0

RX(14) OF 35 COMPOSED OF RX(2), RX(8)

RX(14)       D   +   R   ==>   S



D

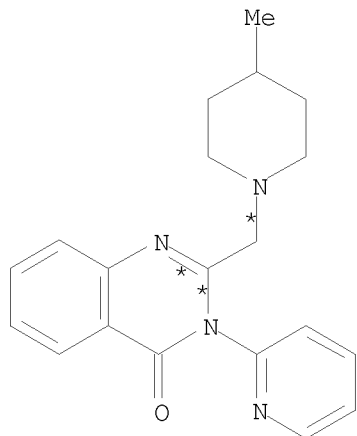


R

2  
STEPS  
→



10/ 562,112



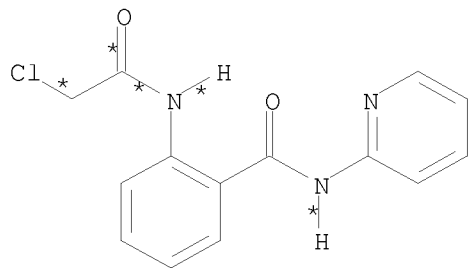
S

RX(2)      RCT   D 96656-50-7  
             PRO   E 76535-05-2  
             CAT   108-24-7 Ac2O

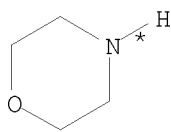
RX(8)      RCT   E 76535-05-2, R 626-58-4  
             PRO   S 96656-54-1

RX(15) OF 35 COMPOSED OF RX(2), RX(9)

RX(15)      D   +   T   ==>   U

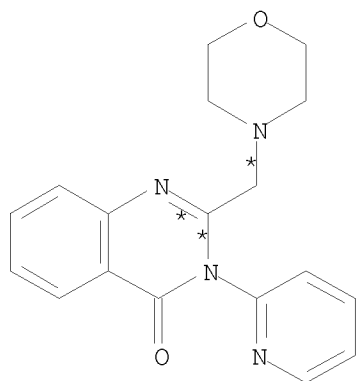


D



T

2  
STEPS  
→

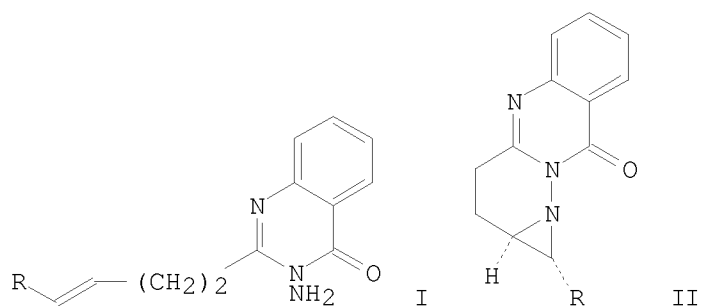


U

RX(2) RCT D 96656-50-7  
 PRO E 76535-05-2  
 CAT 108-24-7 Ac2O

RX(9) RCT E 76535-05-2, T 110-91-8  
 PRO U 96656-55-2

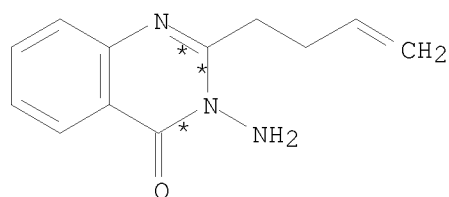
L3 ANSWER 204 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 102:24574 CASREACT  
 TITLE: Intramolecular reactions of N-nitrenes with alkenes  
 AUTHOR(S): Atkinson, Robert S.; Malpass, John R.; Skinner, Karen L.; Woodthorpe, Katherine L.  
 CORPORATE SOURCE: Dep. Chem., Univ. Leicester, Leicester, LE1 7RH, UK  
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1984), (8), 1905-12  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



A

(1)  $\longrightarrow$

Chemical structure of compound A: A benzene ring with a prop-1-en-1-yl group at position 1 and a methyl ester group at position 2. The prop-1-en-1-yl group is labeled with an asterisk on the carbonyl carbon and the nitrogen atom. The methyl ester group is labeled with an asterisk on the carbonyl carbon.

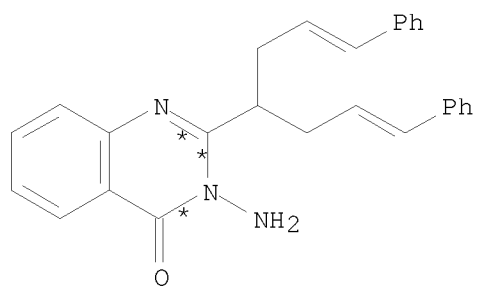


RX(1)	RCT	A 93681-77-7
	RGT	C 302-01-2 N2H4
	PRO	B 79091-40-0
	SOL	67-56-1 MeOH

I

(3)  $\rightarrow$

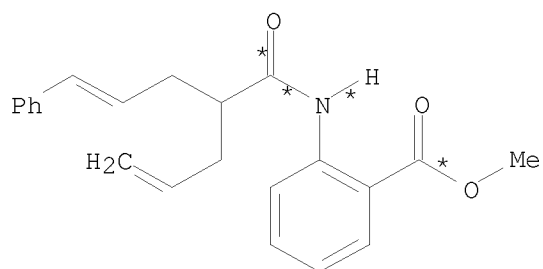
10/ 562,112



J  
YIELD 65%

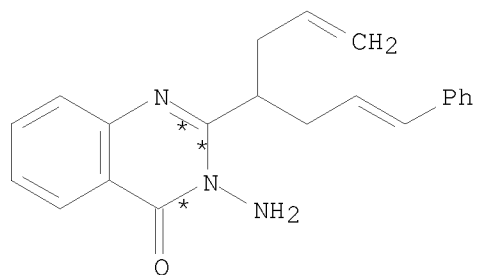
RX(3)	RCT	I	93681-78-8
	RGT	C	302-01-2 N2H4
	PRO	J	79091-43-3

RX(4) OF 21      ...K ==> L



K

(4) >

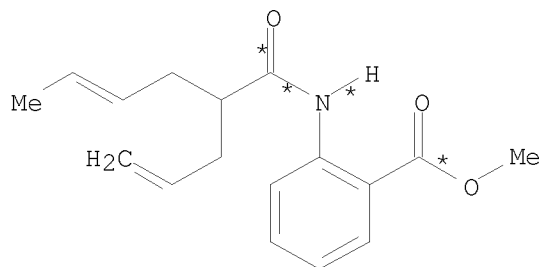


L  
YIELD 50%

RX(4)	RCT	K	93681-79-9
	RGT	C	302-01-2 N2H4
	PRO	L	79091-45-5

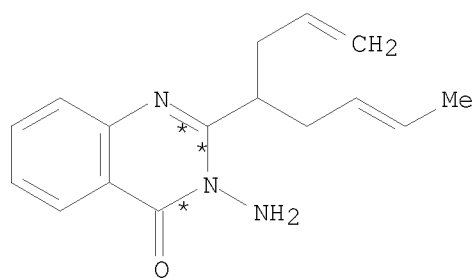
10/ 562,112

RX(5) OF 21 ...M ==> N



M

(5) >

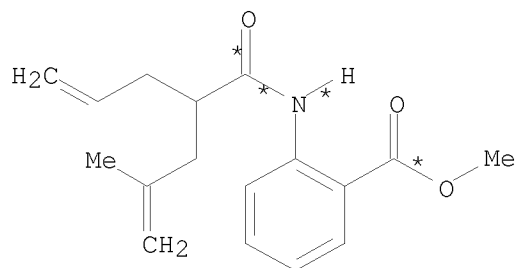


N

YIELD 65%

RX(5) RCT M 93681-80-2  
RGT C 302-01-2 N2H4  
PRO N 79091-46-6

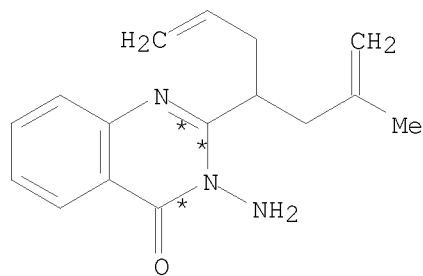
RX(6) OF 21 O ==> P



O

(6) >

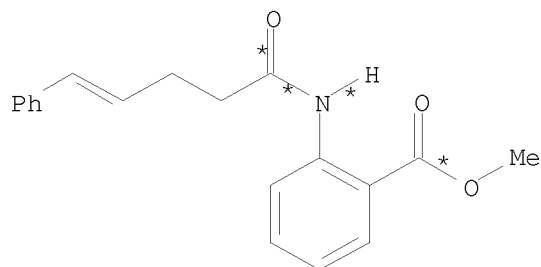
10/ 562,112



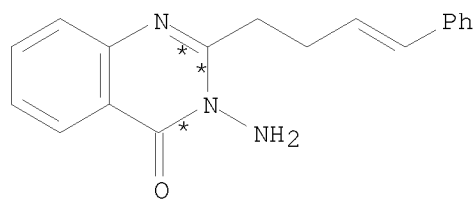
P  
YIELD 73%

RX(6)      RCT   O 93681-81-3  
             RGT   C 302-01-2 N2H4  
             PRO   P 79091-47-7

RX(7) OF 21      ...Q ==> R



Q

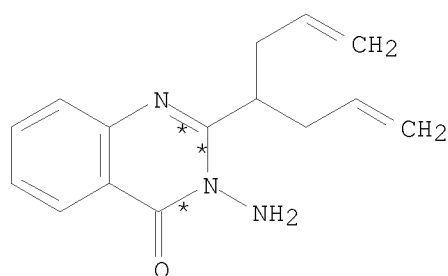
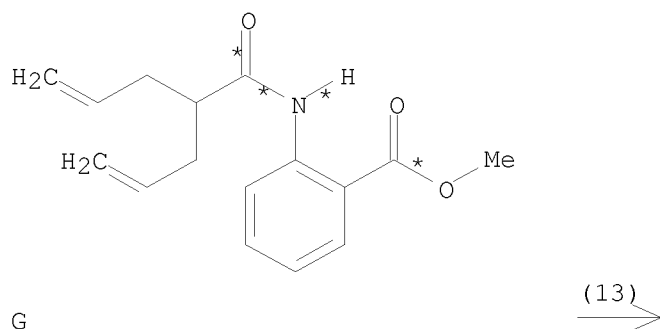


R

RX(7)      RCT   Q 93681-76-6  
             RGT   C 302-01-2 N2H4  
             PRO   R 79091-39-7  
             SOL   67-56-1 MeOH

RX(13) OF 21      ...G ==> X

10/ 562,112



YIELD 85%

RX(13) RCT G 93698-03-4  
RGT C 302-01-2 N2H4  
PRO X 79091-44-4

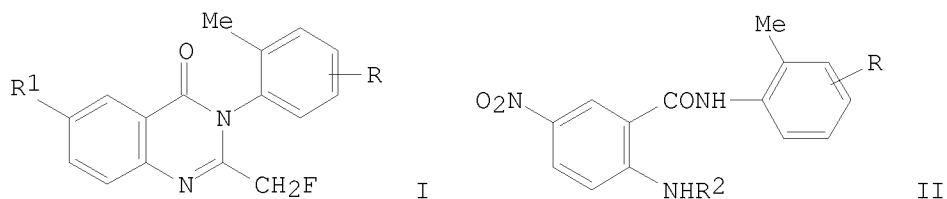
L3 ANSWER 205 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 102:6537 CASREACT  
TITLE: 2-Fluoromethyl-3-(2-methylphenyl)-6-amino-4(3H)-quinazolinones  
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 59128376	A	19840724	JP 1983-4707	19830113
JP 03004074	B	19910122		
EP 116268	A1	19840822	EP 1984-100011	19840102
EP 116268	B1	19880608		
R: BE, CH, DE, FR, GB, IT, LI, NL				
ZA 8400084	A	19840829	ZA 1984-84	19840105

10/ 562,112

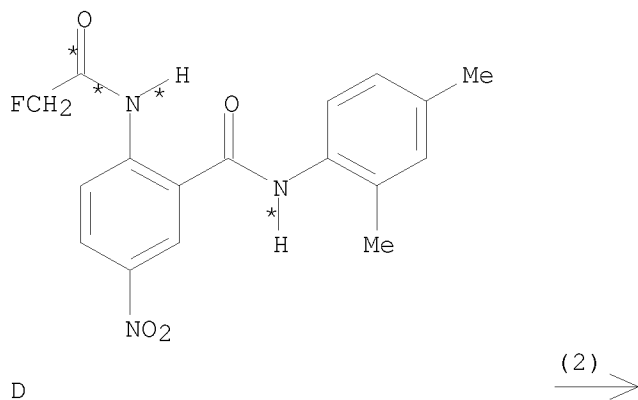
CA 1218367	A1	19870224	CA 1984-445009	19840110
US 4714702	A	19871222	US 1986-888631	19860721
PRIORITY APPLN. INFO.:			JP 1983-4707	19830113
			US 1983-564006	19831221

OTHER SOURCE(S):            MARPAT 102:6537  
GI

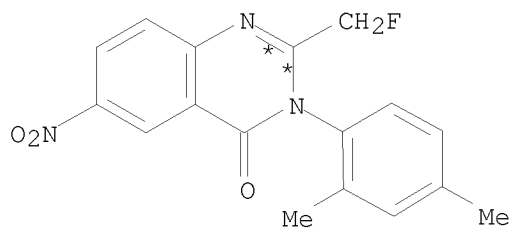


AB The title compds. (I; R = 4-Me, 4-Cl, 3-Me, 4-F, 4-Br, 4-MeO, 5-F, 5-Cl; R<sup>1</sup> = H<sub>2</sub>N) were prepared by acylation of II (R<sup>2</sup> = H) with FCH<sub>2</sub>COX (X = halo), cyclization of the resulting II (R<sup>2</sup> = FCH<sub>2</sub>CO), and reduction of the resulting I (R<sup>1</sup> = O<sub>2</sub>N). Thus, stirring 4 g II (R = 4-Me, R<sup>2</sup> = H) with 2.18 g FCH<sub>2</sub>COCl in THF containing 2.36 g pyridine at room temperature gave 4.3 g II (R = 4-Me, R<sup>2</sup> = FCH<sub>2</sub>CO), which (4 g) was heated with 3.5 g BF<sub>3</sub>-Et<sub>2</sub>O in AcOH at 100-105° to give 2.6 g I (R = 4-Me, R<sup>1</sup> = O<sub>2</sub>N) (III). Reduction of 2 g III with SnCl<sub>2</sub> in MeOH at room temperature gave 1.2 g I (R = 4-Me, R<sup>1</sup> = H<sub>2</sub>N). I (R = 4-Cl) was a more potent muscle relaxant than mephenesin in mice.

RX(2) OF 4        D ==> E...

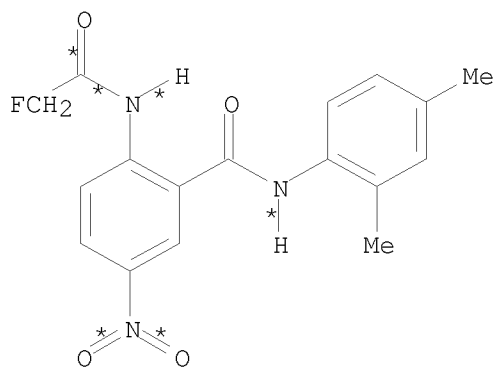






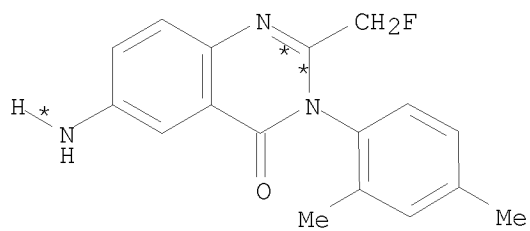
E

RX (2)	RCT	D	93670-44-1
	PRO	E	93670-45-2

$$\begin{array}{lcl} \text{RX}(4) & \text{OF 4 COMPOSED OF} & \text{RX}(2), \text{RX}(3) \\ \text{RX}(4) & \text{D} & \implies \text{F} \end{array}$$


D

2  
STEPS  
→

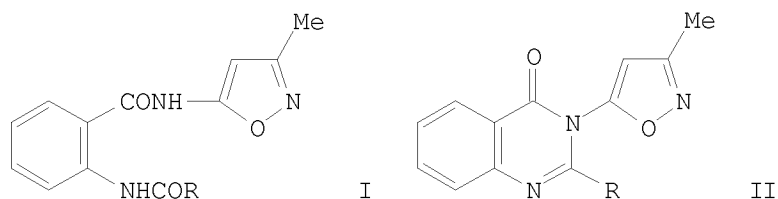


F

RX (2)	RCT	D	93670-44-1
	PRO	E	93670-45-2

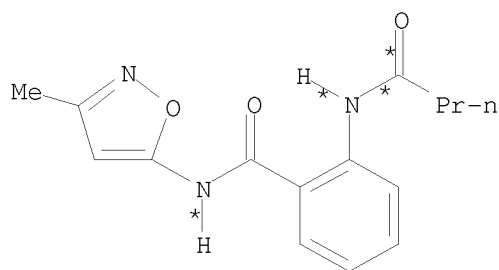
RX (3)	RCT	E	93670-45-2
	PRO	F	93670-47-4

L3 ANSWER 206 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 100:191825 CASREACT  
 TITLE: 3-Isoxazolyl-substituted 4(3H)-quinazolinones of pharmaceutical interest  
 AUTHOR(S): Plescia, S.; Daidone, G.; Ceraulo, L.; Bajardi, M. L.; Reina, R. Arrigo  
 CORPORATE SOURCE: Ist. Chim. Farm. Tossicol., Univ. Palermo, Palermo, Italy  
 SOURCE: Farmaco, Edizione Scientifica (1984), 39(2), 120-4  
 CODEN: FRPSAX; ISSN: 0430-0920  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Italian  
 GI



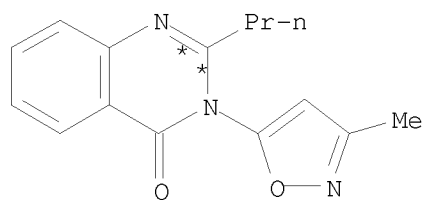
AB Anthranilamides I (R = alkyl; Ph; chloro-, nitro-, or methylphenyl; furyl) were converted to quinazolinones II, useful as analgesics and antiinflammatory and body temperature-lowering agents (no data). Thus, I (R = Pr) was heated with POCl<sub>3</sub> and some water to give II (R = Pr). Anthranilic acid N-(3-methyl-5-isoxazolyl)amide was acylated by RCOCl in pyridine to yield I.

RX(1) OF 30 ...A ==> B



(1)  $\longrightarrow$

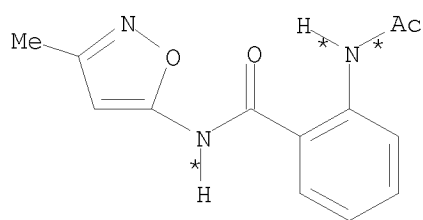
10/ 562,112



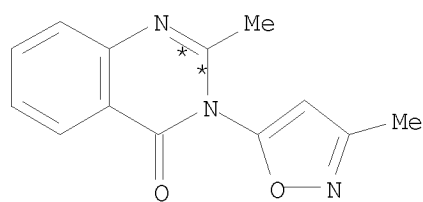
B  
YIELD 28%

RX(1)      RCT    A 90059-30-6  
             RGT    C 10025-87-3 POC13  
             PRO    B 90059-38-4

RX(3) OF 30      ...F ==> G



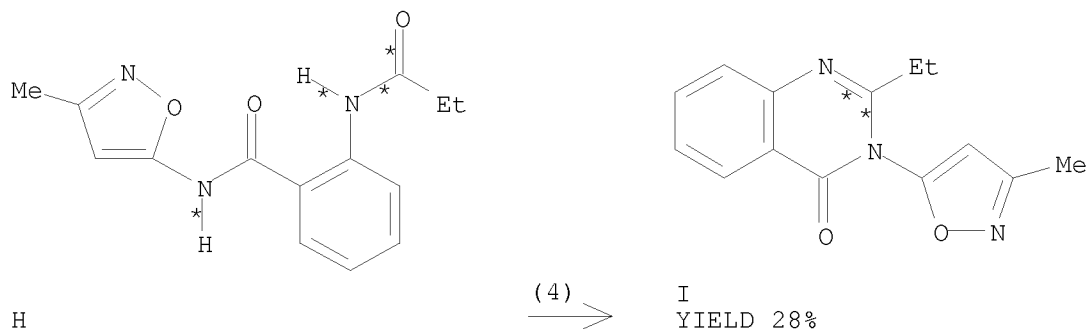
F



G  
YIELD 28%

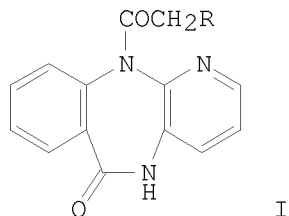
RX(3)      RCT    F 90059-29-3  
             RGT    C 10025-87-3 POC13  
             PRO    G 86134-19-2

RX(4) OF 30      ...H ==> I



RX(4) RCT H 344872-88-4  
RGT C 10025-87-3 POC13  
PRO I 86134-20-5

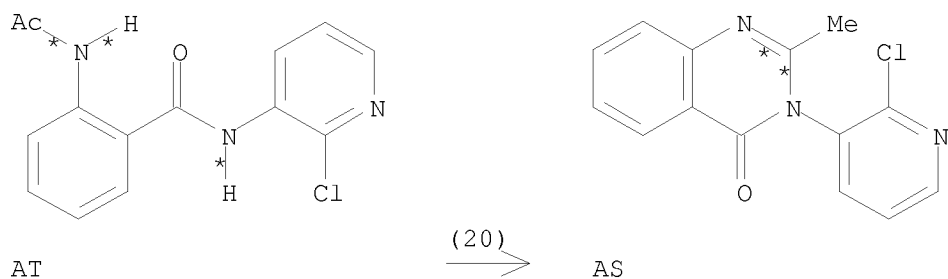
L3 ANSWER 207 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 100:34516 CASREACT  
TITLE: New synthesis of  
11-acyl-5,11-dihydro-6H-pyrido[2,3-b][1,4]benzodiazepin-6-ones and related studies  
AUTHOR(S): Kovac, T.; Oklobdzija, M.; Comisso, G.; Decorte, E.; Fajdiga, T.; Moimas, F.; Angeli, C.; Zonno, F.; Toso, R.; Sunjic, V.  
CORPORATE SOURCE: Chem. Res. Co., San Giovanni, Italy  
SOURCE: Journal of Heterocyclic Chemistry (1983), 20(5), 1339-49  
CODEN: JHTCAD; ISSN: 0022-152X  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB 11-Acyl-5,11-dihydro-6H-pyrido[2,3-b][1,4]benzodiazepin-6-ones I (R = 4-methylpiperazino, imidazolo, 2-methylimidazolo) were prepared via N- $\alpha$ -chloroacetylation and aminolysis. Other attempts at cyclization to form I are also reported.

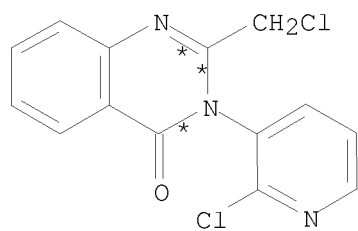
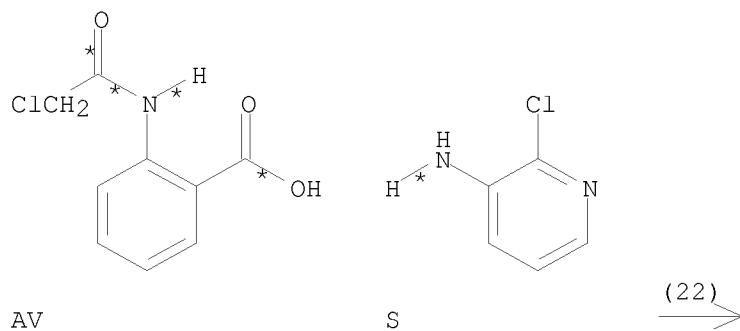
RX(20) OF 178 ...AT ==> AS...

10/ 562,112



RX(20) RCT AT 88369-52-2  
PRO AS 20091-81-0

RX(22) OF 178 AV + S ==> AW...

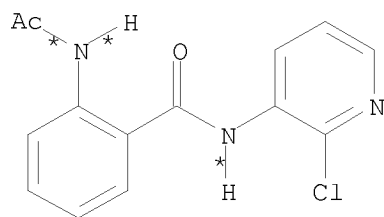


AW  
YIELD 93%

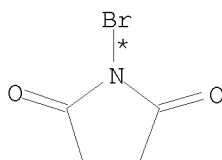
RX(22) RCT AV 14422-49-2, S 6298-19-7  
PRO AW 88369-53-3

RX(69) OF 178 COMPOSED OF RX(20), RX(23)  
RX(69) AT + AX ==> AY

10/ 562,112

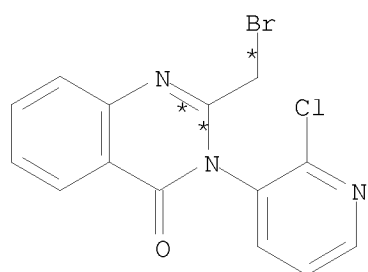


AT



AX

2  
STEPS  
→

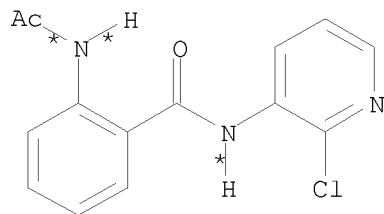


AY

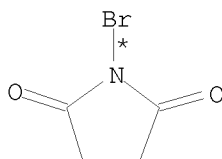
RX(20) RCT AT 88369-52-2  
PRO AS 20091-81-0

RX(23) RCT AS 20091-81-0, AX 128-08-5  
PRO AY 88369-54-4  
CAT 78-67-1 AIBN

RX(70) OF 178 COMPOSED OF RX(20), RX(47)  
RX(70) AT + 2 AX ==> BY



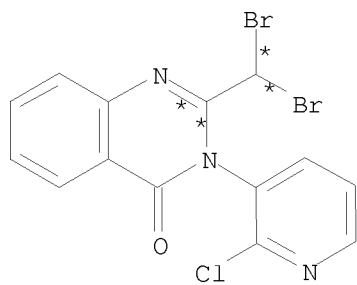
AT



2 AX

2  
STEPS  
→

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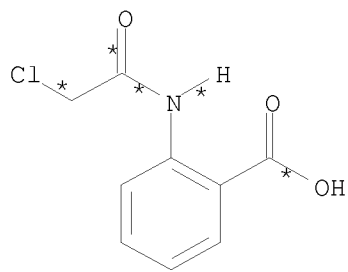


BY

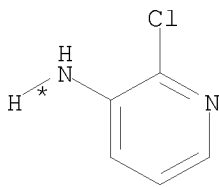
RX(20) RCT AT 88369-52-2  
PRO AS 20091-81-0

RX(47) RCT AS 20091-81-0, AX 128-08-5  
PRO BY 344868-00-4  
CAT 78-67-1 AIBN

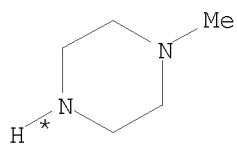
RX(72) OF 178 COMPOSED OF RX(22), RX(24)  
RX(72) AV + S + AP ==> BA



AV



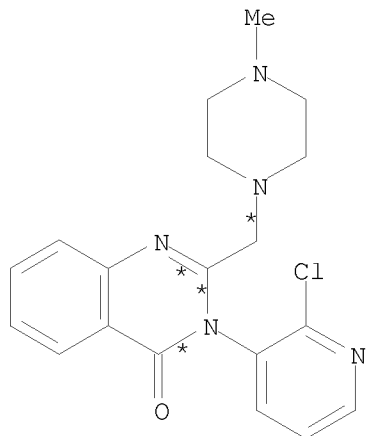
S



AP

2  
STEPS  
→

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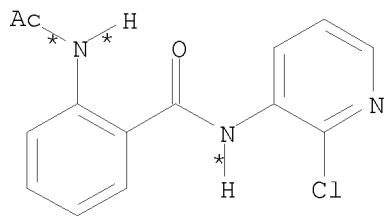


BA

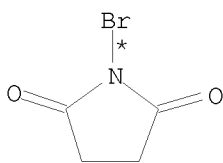
RX(22) RCT AV 14422-49-2, S 6298-19-7  
PRO AW 88369-53-3

RX(24) RCT AW 88369-53-3, AP 109-01-3  
PRO BA 88369-55-5

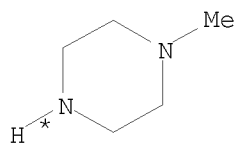
RX(110) OF 178 COMPOSED OF RX(20), RX(23), RX(25)  
RX(110) AT + AX + AP ==> BA



AT



AX

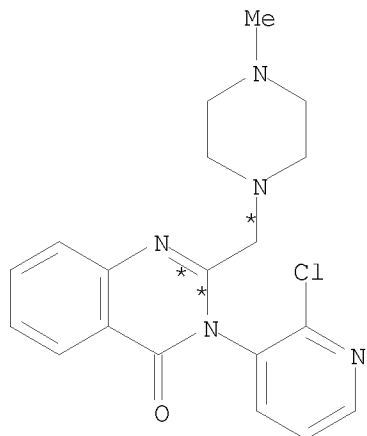


AP

3  
STEPS  
→



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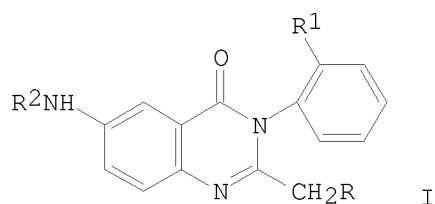
BA  
YIELD 90%

RX(20) RCT AT 88369-52-2  
PRO AS 20091-81-0

RX(23) RCT AS 20091-81-0, AX 128-08-5  
PRO AY 88369-54-4  
CAT 78-67-1 AIBN

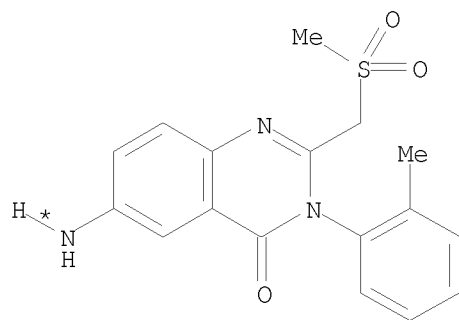
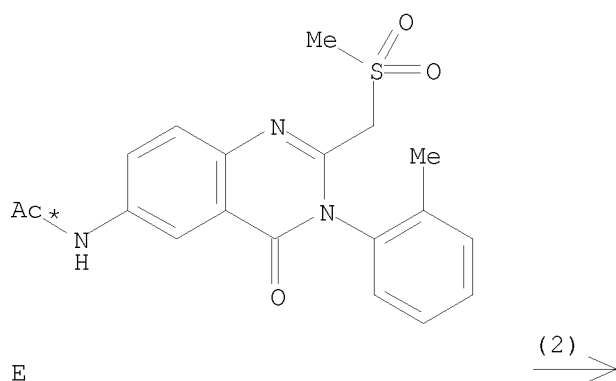
RX(25) RCT AY 88369-54-4, AP 109-01-3  
PRO BA 88369-55-5

L3 ANSWER 208 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 99:139890 CASREACT  
TITLE: Synthesis of the metabolites of afloqualone and related compounds  
AUTHOR(S): Yamada, Yoshihisa; Otsuka, Minezo; Tani, Junichi; Oine, Toyonari  
CORPORATE SOURCE: Res. Lab. Appl. Biochem., Tanabe Seiyaku Co., Ltd., Osaka, 532, Japan  
SOURCE: Chemical & Pharmaceutical Bulletin (1983), 31(4), 1158-65  
CODEN: CPBTAL; ISSN: 0009-2363  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Seven main metabolites I [R = F, SMe, SO<sub>2</sub>Me, SCH<sub>2</sub>CH(NHAc)CO<sub>2</sub>H, OH; R<sub>1</sub> = Me, CH<sub>2</sub>OH; R<sub>2</sub> = Ac, COCH<sub>2</sub>OH] of afloqualone (I, R = F, R<sub>1</sub> = Me, R<sub>2</sub> = H) and related 4(3H)-quinazolinone derivs. were synthesized. I (R = SMe, SO<sub>2</sub>Me, R<sub>1</sub> = Me, R<sub>2</sub> = Ac) were prepared by the reaction of I (R = Cl, R<sub>1</sub> = Me, R<sub>2</sub> = Ac) with NaSMe followed by oxidation with H<sub>2</sub>O<sub>2</sub>. Reaction of I (R = Cl, R<sub>1</sub> = Me, R<sub>2</sub> = Ac) and N-acetylcysteine gave I [R = SCH<sub>2</sub>CH(NHAc)CO<sub>2</sub>H, R<sub>1</sub> = Me, R<sub>2</sub> = Ac]. Condensation of 2-fluoroacetamido-5-nitrobenzoic acid and 2-aminobenzyl alc. with dicyclohexylcarbodiimide in the presence of 1-hydroxybenzotriazole afforded 2-fluoromethyl-3-(o-hydroxymethylphenyl)-6-nitro-4(3H)-quinazolinone, which was converted to I (R = F, R<sub>1</sub> = CH<sub>2</sub>OH, R<sub>2</sub> = Ac, COCH<sub>2</sub>OH). Treatment of I (R = Br, R<sub>1</sub> = Me, R<sub>2</sub> = Ac) with AgBF<sub>4</sub>.H<sub>2</sub>O in Me<sub>2</sub>SO gave I (R = OH, R<sub>1</sub> = Me, R<sub>2</sub> = Ac). None of the main metabolites showed significant central nervous system depressant activity.

RX(2) OF 41 ...E ==> F

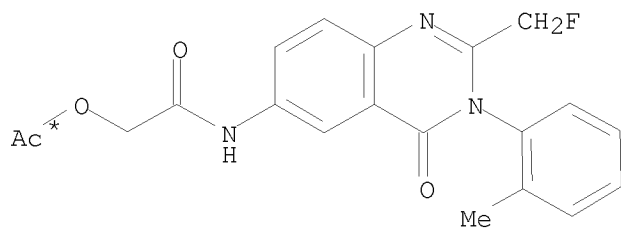


F  
YIELD 69%

RX(2) RCT E 87266-00-0  
RGT D 7647-01-0 HCl  
PRO F 87266-03-3

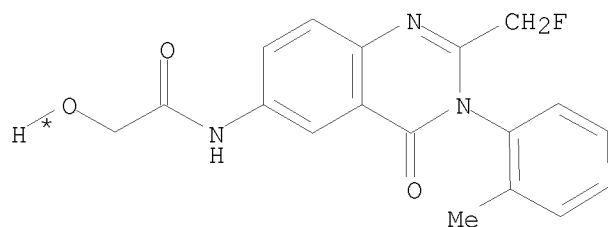
RX(4) OF 41 ...I ==> J

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I

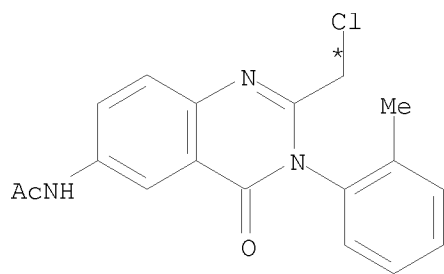
(4)  $\longrightarrow$



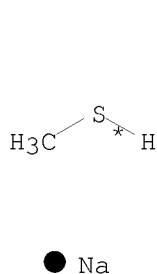
J

RX(4)      RCT    I 87265-98-3  
               PRO    J 87081-79-6  
               CAT    144-55-8 NaHCO<sub>3</sub>

RX(6) OF 41      M + N ==> O...



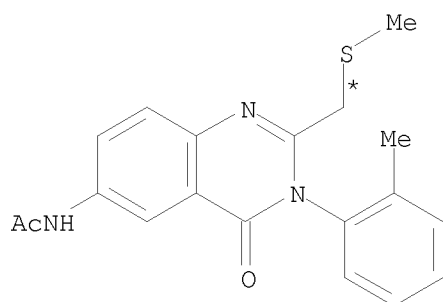
M



N

(6)  $\longrightarrow$

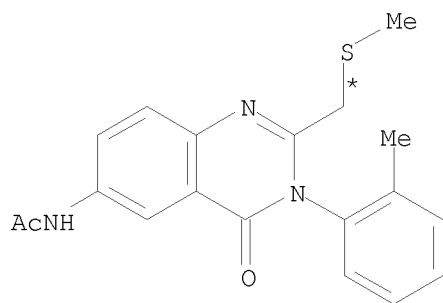
10/ 562,112



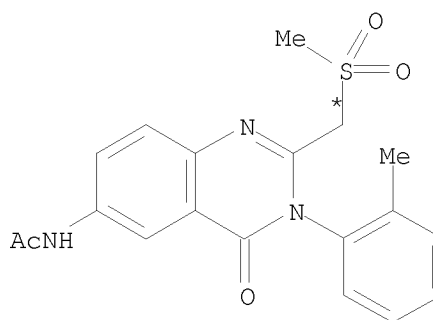
O  
YIELD 92%

RX(6) RCT M 61899-78-3, N 5188-07-8  
PRO O 87265-99-4

RX(7) OF 41 ...O ==> E...



O

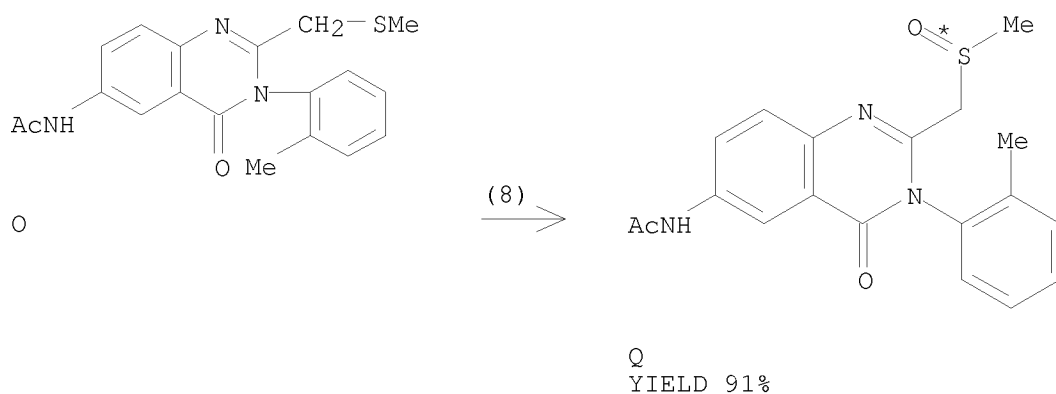


E  
YIELD 48%

RX(7) RCT O 87265-99-4  
RGT P 7722-84-1 H2O2  
PRO E 87266-00-0

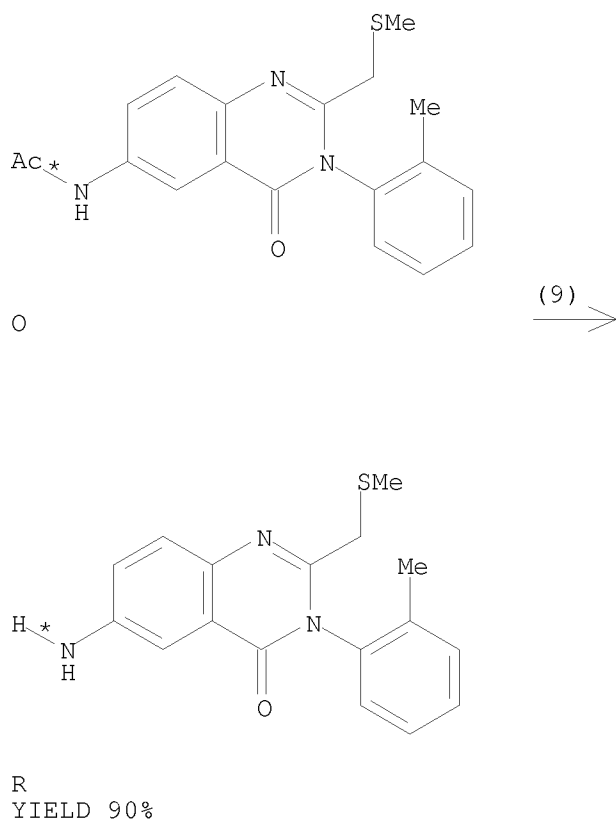
RX(8) OF 41 ...O ==> Q

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RX(8)      RCT    O 87265-99-4  
              RGT    P 7722-84-1 H2O2  
              PRO    Q 87266-01-1

RX(9) OF 41      ...O ==> R...

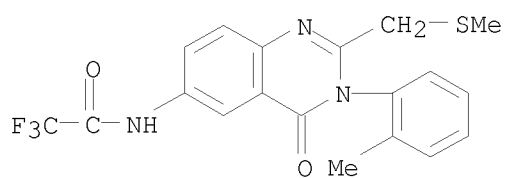


RX(9)      RCT    O 87265-99-4  
              RGT    D 7647-01-0 HCl

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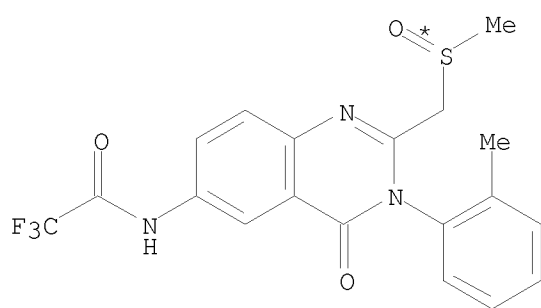
PRO R 87266-02-2

RX(11) OF 41 ...T ==> U...



T

(11)

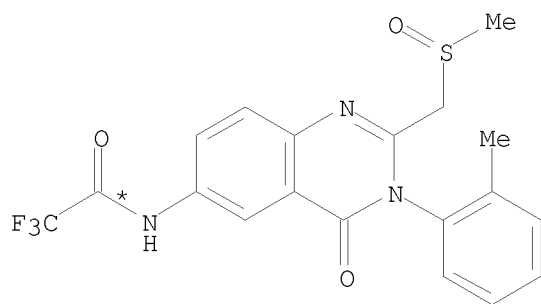


U

YIELD 77%

RX(11) RCT T 87266-05-5  
RGT P 7722-84-1 H2O2  
PRO U 87266-06-6

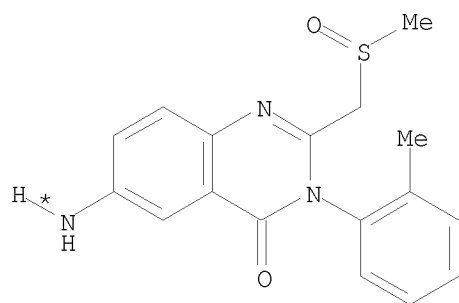
RX(12) OF 41 ...U ==> V



U

(12)

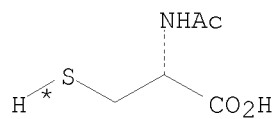
10/ 562,112



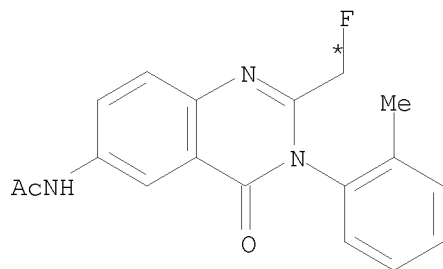
V

RX(12)      RCT    U 87266-06-6  
               PRO    V 87266-07-7  
               CAT    67-56-1 MeOH

RX(13) OF 41      X    +    Y    ==>    Z...



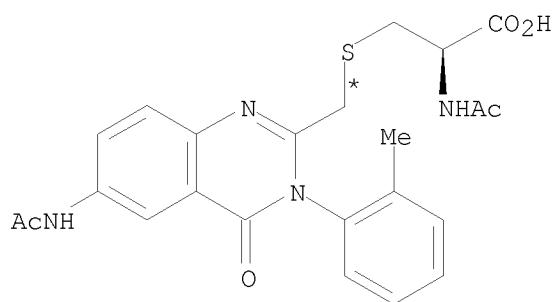
X



Y

(13)

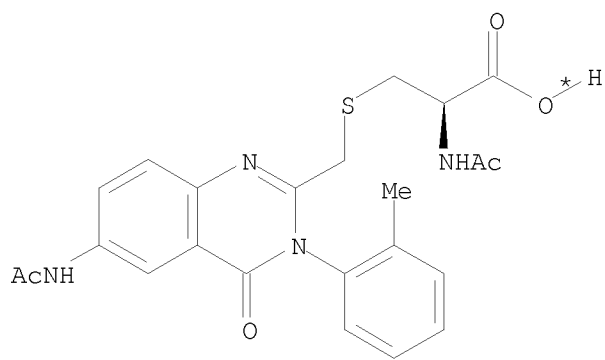
10/ 562,112



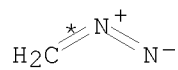
Z  
YIELD 92%

RX(13)      RCT    X 616-91-1, Y 61899-79-4  
              PRO    Z 87266-09-9

RX(14) OF 41      ...Z    +    AA    ==>    AB



Z

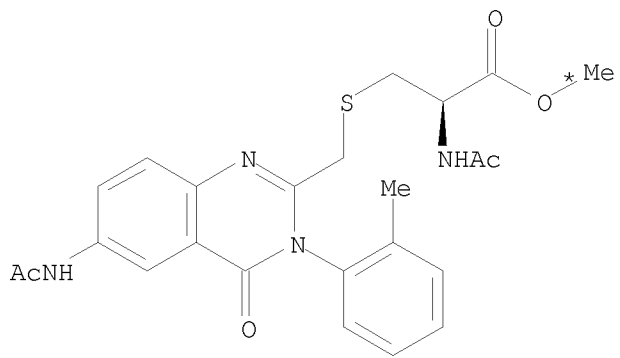


AA

(14)  
→



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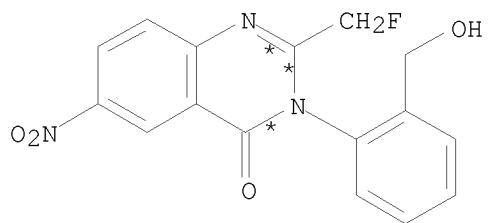
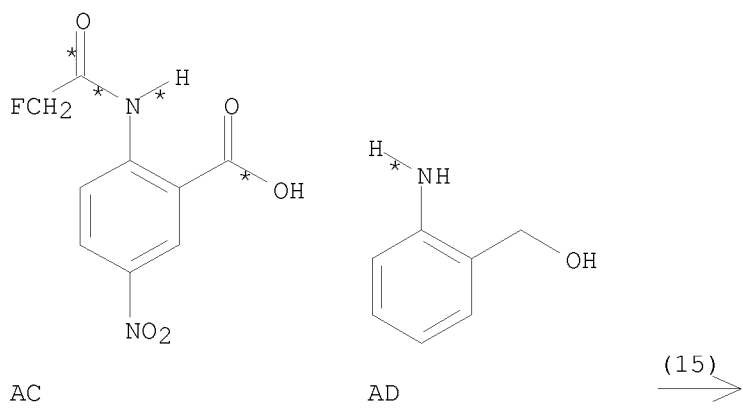


AB

YIELD 87%

RX(14) RCT Z 87266-09-9, AA 334-88-3  
PRO AB 87266-08-8

RX(15) OF 41 AC + AD ==> A...



A

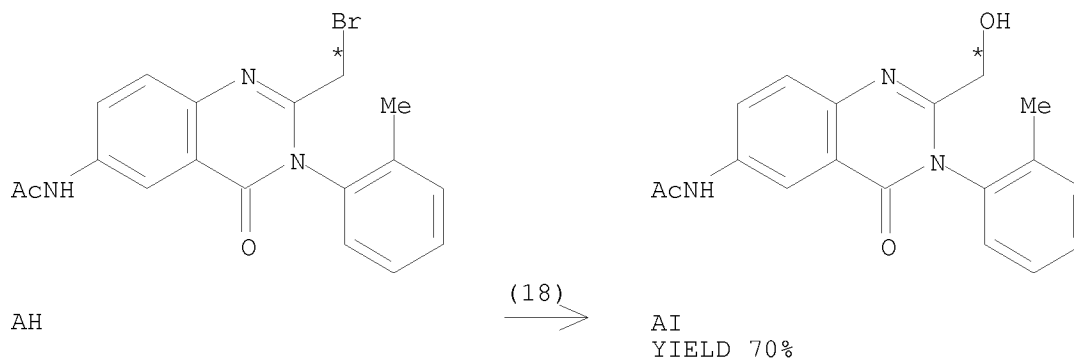
YIELD 25%

RX(15) RCT AC 87266-10-2, AD 5344-90-1

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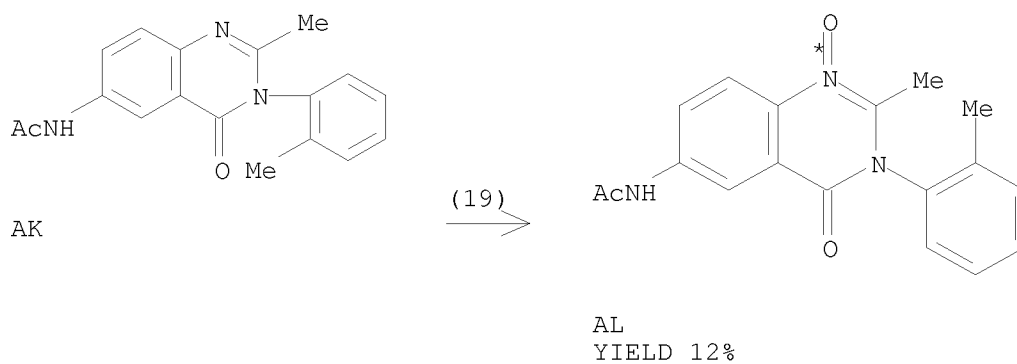
PRO A 87266-11-3

RX(18) OF 41 AH ==> AI



RX(18) RCT AH 87266-12-4  
RGT AJ 14104-20-2 AgBF<sub>4</sub>  
PRO AI 87266-13-5

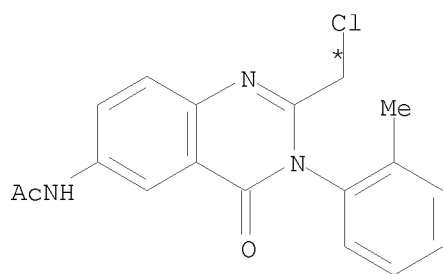
RX(19) OF 41 AK ==> AL



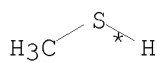
RX(19) RCT AK 1096-46-4  
RGT P 7722-84-1 H<sub>2</sub>O<sub>2</sub>  
PRO AL 87266-14-6

RX(24) OF 41 COMPOSED OF RX(6), RX(7)  
RX(24) M + N ==> E

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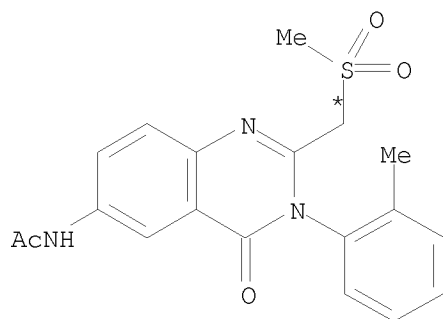


M



N

2  
STEPS  
→



E

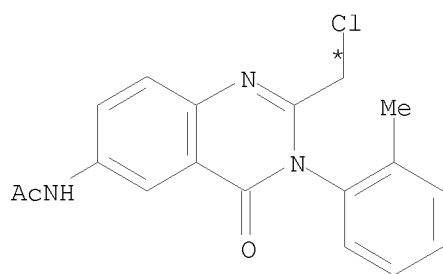
YIELD 48%

RX(6) RCT M 61899-78-3, N 5188-07-8  
PRO O 87265-99-4

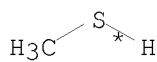
RX(7) RCT O 87265-99-4  
RGT P 7722-84-1 H2O2  
PRO E 87266-00-0

RX(25) OF 41 COMPOSED OF RX(6), RX(8)

RX(25) M + N ==> Q



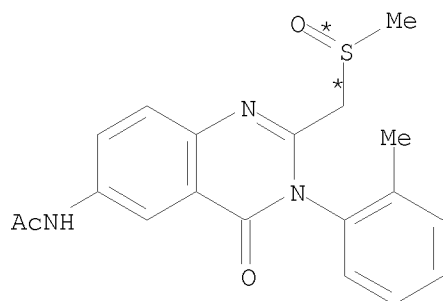
M



N

2  
STEPS  
→

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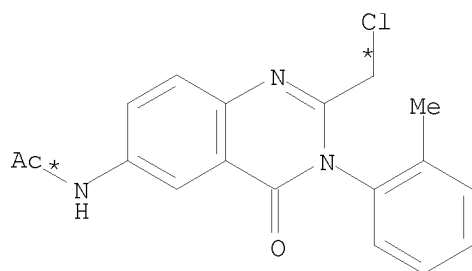


Q  
YIELD 91%

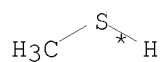
RX(6) RCT M 61899-78-3, N 5188-07-8  
PRO O 87265-99-4

RX(8) RCT O 87265-99-4  
RGT P 7722-84-1 H2O2  
PRO Q 87266-01-1

RX(26) OF 41 COMPOSED OF RX(6), RX(9)  
RX(26) M + N ==> R



M

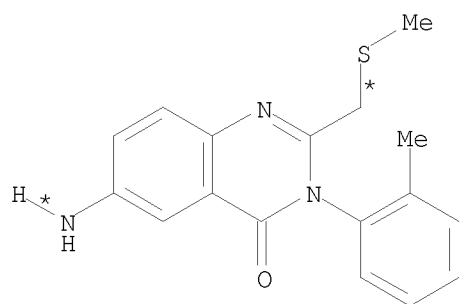


● Na

N

2  
STEPS  
→

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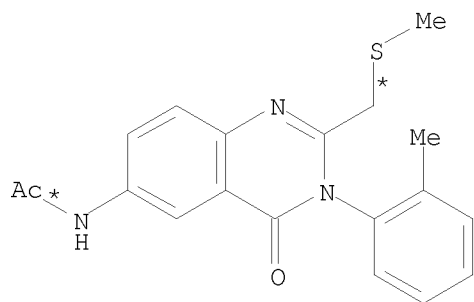


R  
YIELD 90%

RX(6) RCT M 61899-78-3, N 5188-07-8  
PRO O 87265-99-4

RX(9) RCT O 87265-99-4  
RGT D 7647-01-0 HCl  
PRO R 87266-02-2

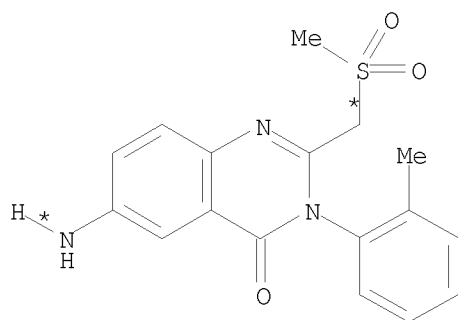
RX(27) OF 41 COMPOSED OF RX(7), RX(2)  
RX(27) O ==> F



O

2  
STEPS  
→

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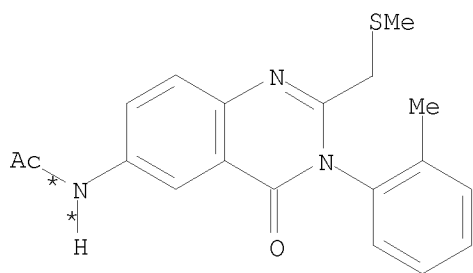


F  
YIELD 69%

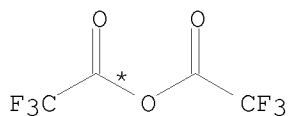
RX(7)      RCT    O 87265-99-4  
             RGT    P 7722-84-1 H2O2  
             PRO    E 87266-00-0

RX(2)      RCT    E 87266-00-0  
             RGT    D 7647-01-0 HCl  
             PRO    F 87266-03-3

RX(28) OF 41 COMPOSED OF RX(9), RX(10)  
RX(28)      O    +    S    ==>    T



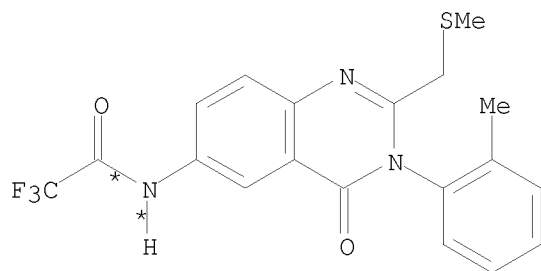
O



S

2  
STEPS  
→

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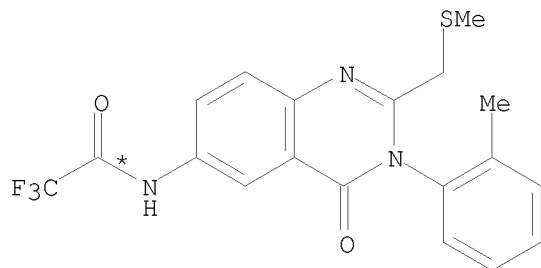


T  
YIELD 95%

RX(9)      RCT   O 87265-99-4  
              RGT   D 7647-01-0 HCl  
              PRO   R 87266-02-2

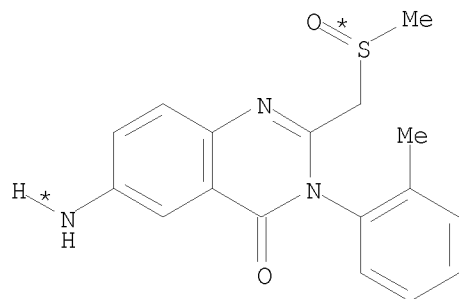
RX(10)      RCT   R 87266-02-2, S 407-25-0  
              PRO   T 87266-05-5

RX(30) OF 41 COMPOSED OF RX(11), RX(12)  
RX(30)      T ==> V



T

2  
STEPS  
→



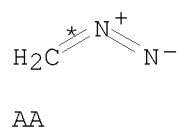
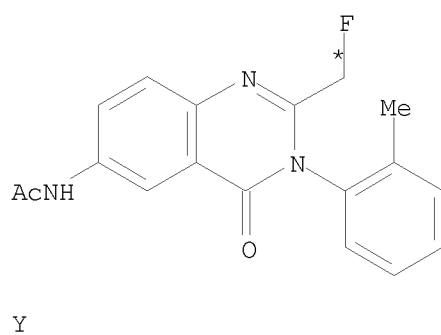
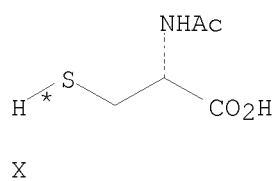
V

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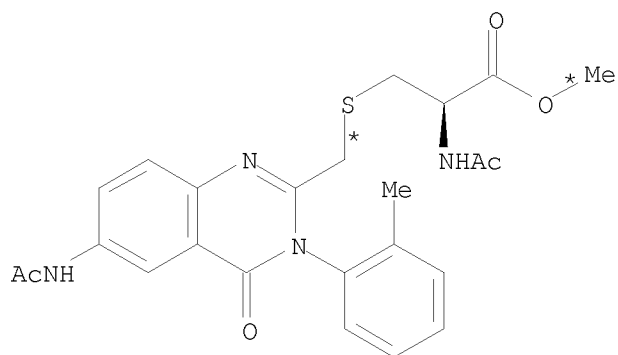
RX(11)      RCT    T 87266-05-5  
              RGT    P 7722-84-1 H2O2  
              PRO    U 87266-06-6

RX(12)      RCT    U 87266-06-6  
              PRO    V 87266-07-7  
              CAT    67-56-1 MeOH

RX(31) OF 41 COMPOSED OF RX(13), RX(14)  
RX(31)      X + Y + AA ==> AB



2  
STEPS  
→



AB  
YIELD 87%

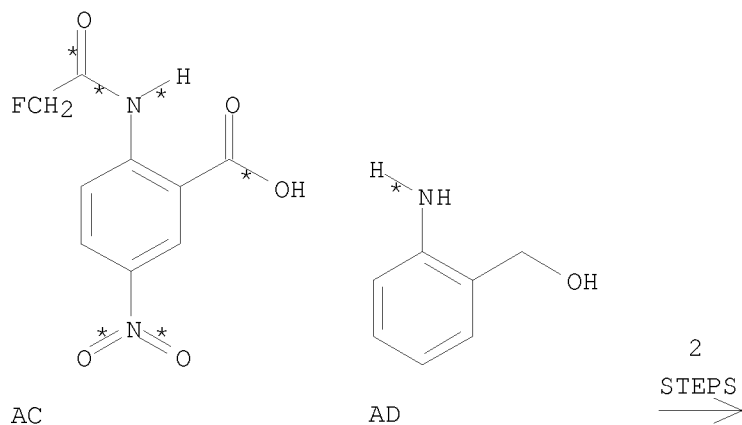
RX(13)      RCT    X 616-91-1, Y 61899-79-4  
              PRO    Z 87266-09-9

RX(14)      RCT    Z 87266-09-9, AA 334-88-3  
              PRO    AB 87266-08-8



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RX(32) OF 41 COMPOSED OF RX(15), RX(1)  
RX(32) AC + AD ==> B



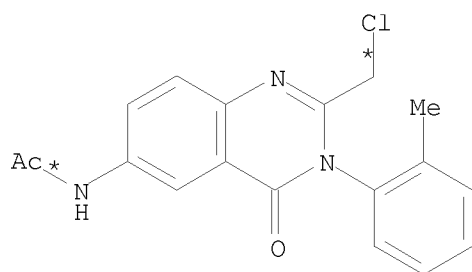
B  
YIELD 64%

RX(15) RCT AC 87266-10-2, AD 5344-90-1  
PRO A 87266-11-3

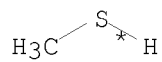
RX(1) RCT A 87266-11-3  
RGT C 7772-99-8 SnCl<sub>2</sub>, D 7647-01-0 HCl  
PRO B 73832-13-0

RX(33) OF 41 COMPOSED OF RX(6), RX(7), RX(2)  
RX(33) M + N ==> F

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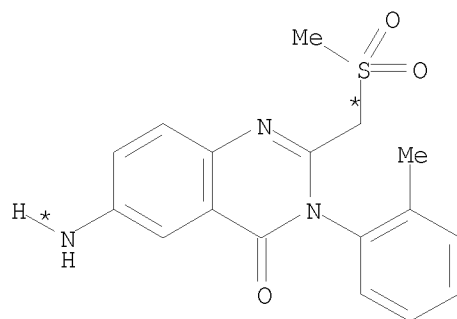


M



N

3  
STEPS  
→



F

YIELD 69%

RX(6) RCT M 61899-78-3, N 5188-07-8  
PRO O 87265-99-4

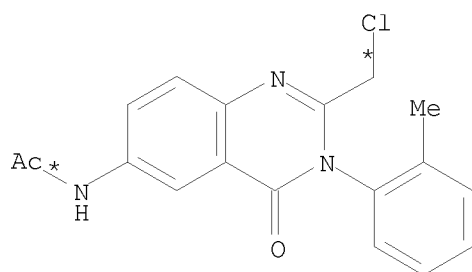
RX(7) RCT O 87265-99-4  
RGT P 7722-84-1 H2O2  
PRO E 87266-00-0

RX(2) RCT E 87266-00-0  
RGT D 7647-01-0 HCl  
PRO F 87266-03-3

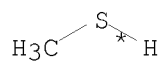
RX(34) OF 41 COMPOSED OF RX(6), RX(9), RX(10)

RX(34) M + N + S ==> T

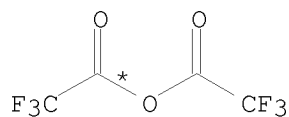
10/ 562,112



M

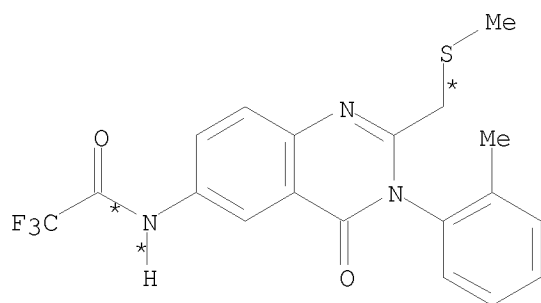


N



S

3  
STEPS  
→



T  
YIELD 95%

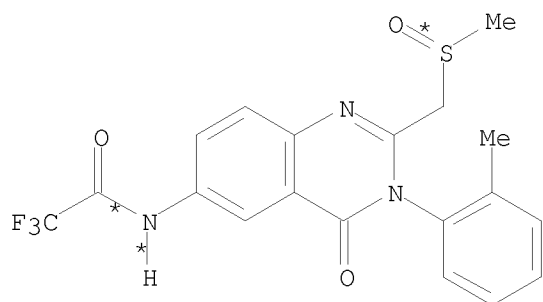
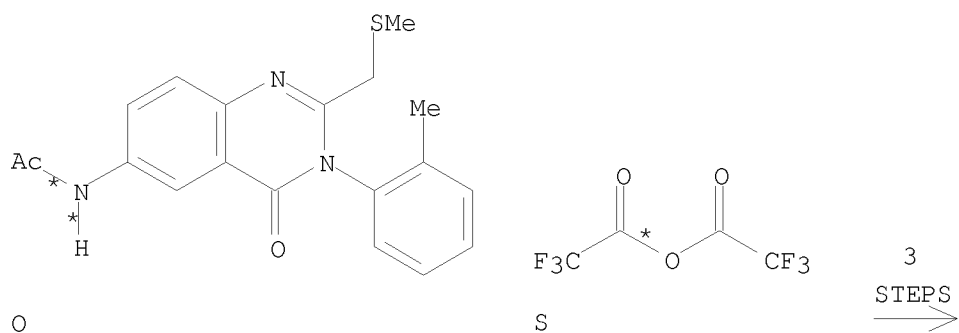
RX(6) RCT M 61899-78-3, N 5188-07-8  
PRO O 87265-99-4

RX(9) RCT O 87265-99-4  
RGT D 7647-01-0 HCl  
PRO R 87266-02-2

RX(10) RCT R 87266-02-2, S 407-25-0  
PRO T 87266-05-5

RX(35) OF 41 COMPOSED OF RX(9), RX(10), RX(11)  
RX(35) O + S ==> U

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U  
YIELD 77%

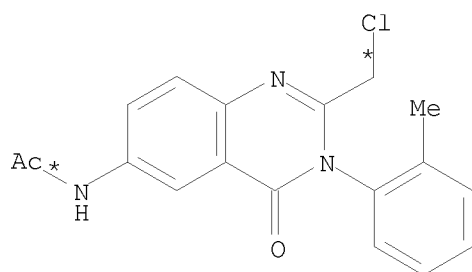
RX(9) RCT O 87265-99-4  
RGT D 7647-01-0 HCl  
PRO R 87266-02-2

RX(10) RCT R 87266-02-2, S 407-25-0  
PRO T 87266-05-5

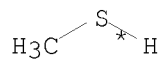
RX(11) RCT T 87266-05-5  
RGT P 7722-84-1 H<sub>2</sub>O<sub>2</sub>  
PRO U 87266-06-6

RX(36) OF 41 COMPOSED OF RX(6), RX(9), RX(10), RX(11)  
RX(36) M + N + S ==> U

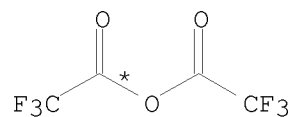
10/ 562,112



M

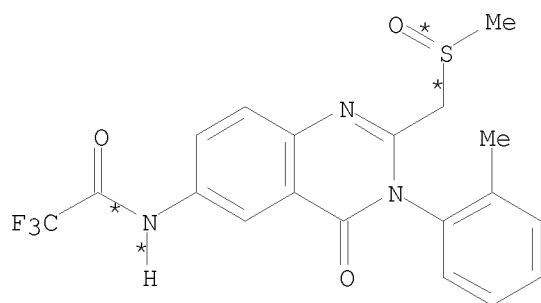


N



S

4  
STEPS  
→



U

YIELD 77%

RX(6) RCT M 61899-78-3, N 5188-07-8  
PRO O 87265-99-4

RX(9) RCT O 87265-99-4  
RGT D 7647-01-0 HCl  
PRO R 87266-02-2

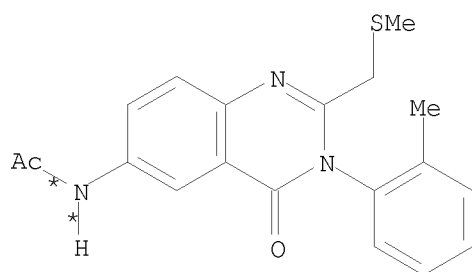
RX(10) RCT R 87266-02-2, S 407-25-0  
PRO T 87266-05-5

RX(11) RCT T 87266-05-5  
RGT P 7722-84-1 H2O2  
PRO U 87266-06-6

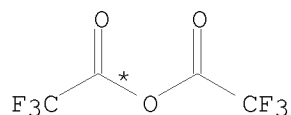
RX(38) OF 41 COMPOSED OF RX(9), RX(10), RX(11), RX(12)

RX(38) O + S ==> V

10/ 562,112

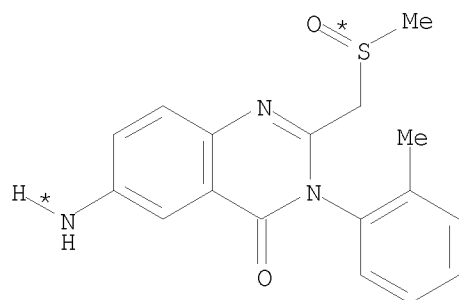


O



S

4  
STEPS  
→



V

RX(9) RCT O 87265-99-4  
RGT D 7647-01-0 HCl  
PRO R 87266-02-2

RX(10) RCT R 87266-02-2, S 407-25-0  
PRO T 87266-05-5

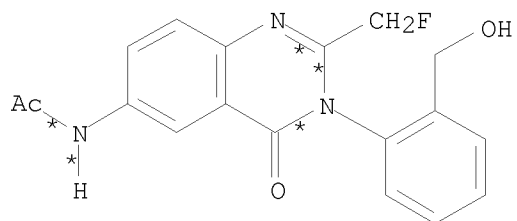
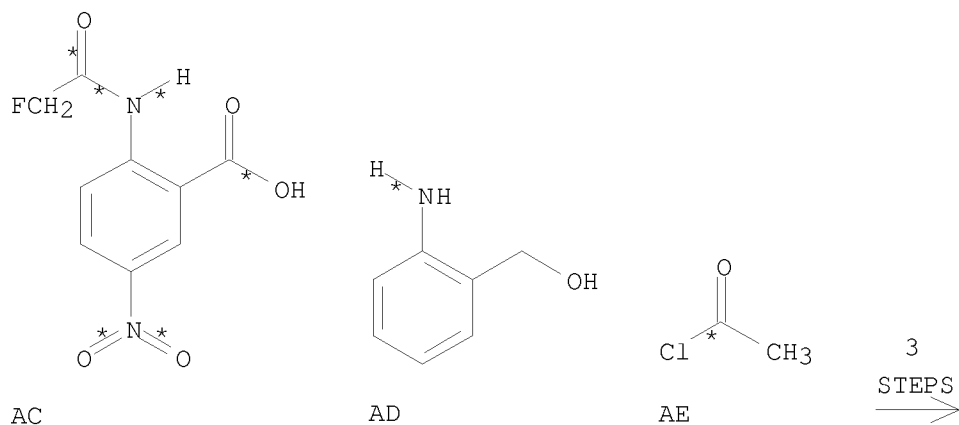
RX(11) RCT T 87266-05-5  
RGT P 7722-84-1 H2O2  
PRO U 87266-06-6

RX(12) RCT U 87266-06-6  
PRO V 87266-07-7  
CAT 67-56-1 MeOH

RX(39) OF 41 COMPOSED OF RX(15), RX(1), RX(16)

RX(39) AC + AD + AE ==> AF

10/ 562,112



AF  
YIELD 92%

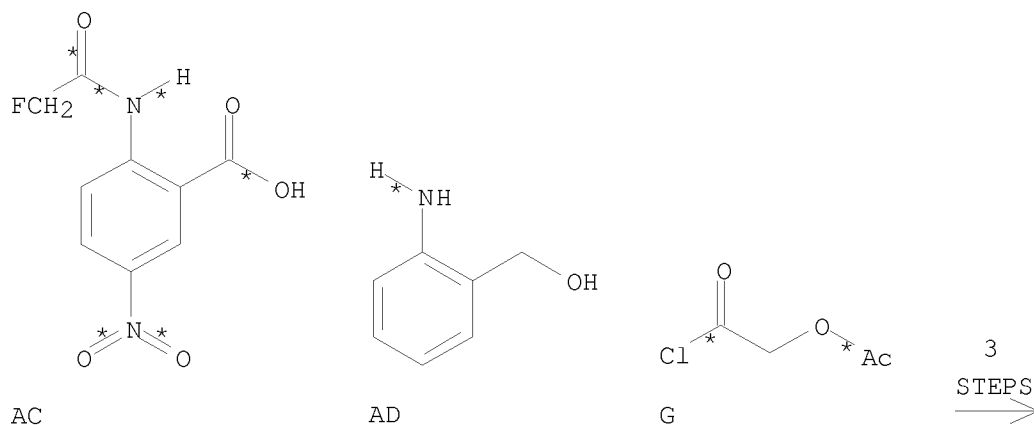
RX(15) RCT AC 87266-10-2, AD 5344-90-1  
PRO A 87266-11-3

RX(1) RCT A 87266-11-3  
RGT C 7772-99-8 SnCl<sub>2</sub>, D 7647-01-0 HCl  
PRO B 73832-13-0

RX(16) RCT B 73832-13-0, AE 75-36-5  
PRO AF 87081-78-5

RX(40) OF 41 COMPOSED OF RX(15), RX(1), RX(17)  
RX(40) AC + AD + G ==> AG

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AG  
YIELD 70%

RX(15) RCT AC 87266-10-2, AD 5344-90-1  
PRO A 87266-11-3

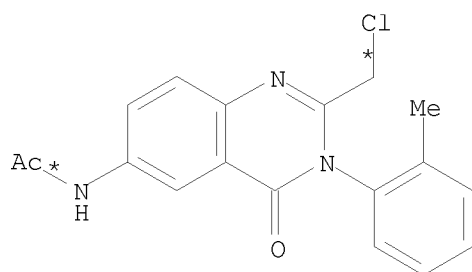
RX(1) RCT A 87266-11-3  
RGT C 7772-99-8 SnCl<sub>2</sub>, D 7647-01-0 HCl  
PRO B 73832-13-0

RX(17) RCT G 13831-31-7, B 73832-13-0  
PRO AG 87081-80-9

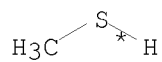
RX(41) OF 41 COMPOSED OF RX(6), RX(9), RX(10), RX(11), RX(12)  
RX(41) M + N + S ==> V



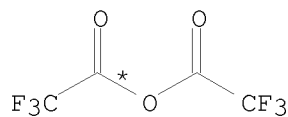
10/ 562,112



M

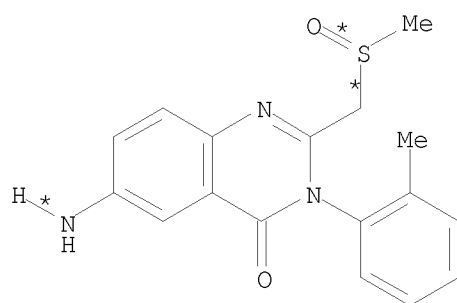


N



S

5  
STEPS  
→



V

RX(6) RCT M 61899-78-3, N 5188-07-8  
PRO O 87265-99-4

RX(9) RCT O 87265-99-4  
RGT D 7647-01-0 HCl  
PRO R 87266-02-2

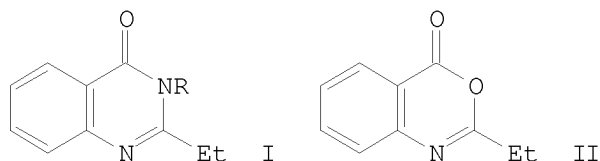
RX(10) RCT R 87266-02-2, S 407-25-0  
PRO T 87266-05-5

RX(11) RCT T 87266-05-5  
RGT P 7722-84-1 H2O2  
PRO U 87266-06-6

RX(12) RCT U 87266-06-6  
PRO V 87266-07-7  
CAT 67-56-1 MeOH

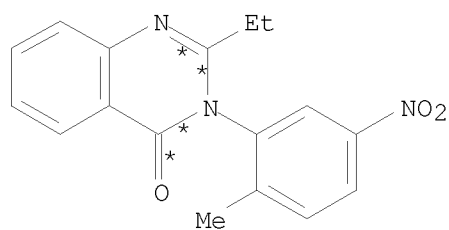
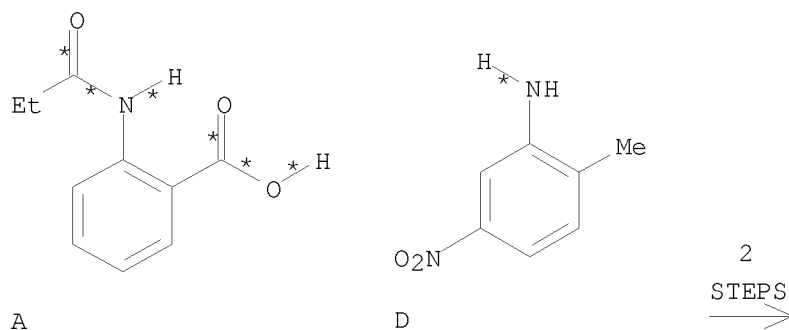
10/ 562,112

L3 ANSWER 209 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 98:198154 CASREACT  
TITLE: Synthesis and properties of  
2-ethyl-3-aryl(arylamino)-4(3H)-quinazolinones  
AUTHOR(S): Smirnova, N. N.; Kozhevnikov, Yu. V.  
CORPORATE SOURCE: Perm. Gos. Farm. Inst., Perm, USSR  
SOURCE: Deposited Doc. (1982), VINITI 1613-82, 7 pp. Avail.:  
VINITI  
DOCUMENT TYPE: Report  
LANGUAGE: Russian  
GI



AB The title compds. I [R = 2,5-Me(O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>, 2,4-(O<sub>2</sub>N)MeC<sub>6</sub>H<sub>3</sub>, 2,5-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, PhNH, o-, m-, p-MeC<sub>6</sub>H<sub>4</sub>NH, p-BrC<sub>6</sub>H<sub>4</sub>NH] were prepared in 25-75% yields by cyclocondensation of II with RNH<sub>2</sub>.

RX(10) OF 17 COMPOSED OF RX(1), RX(2)  
RX(10) A + D ==> E



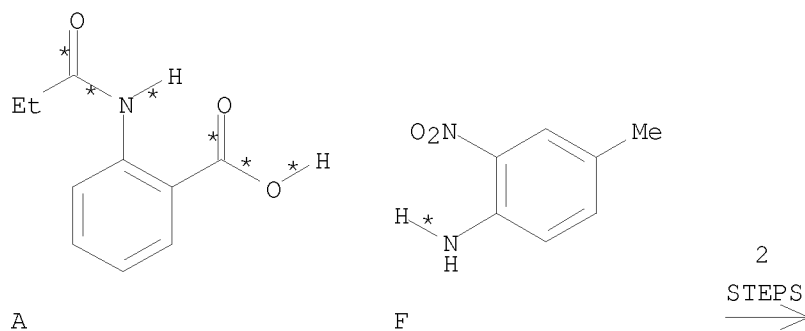
E  
YIELD 64%

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RX(1)        RCT    A 19165-26-5  
              PRO    B 2916-09-8  
              CAT    75-07-0 MeCHO

RX(2)        RCT    B 2916-09-8, D 99-55-8  
              PRO    E 85731-86-8

RX(11) OF 17 COMPOSED OF RX(1), RX(3)  
RX(11)       A    +    F    ==>    G



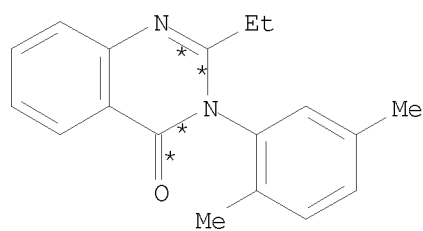
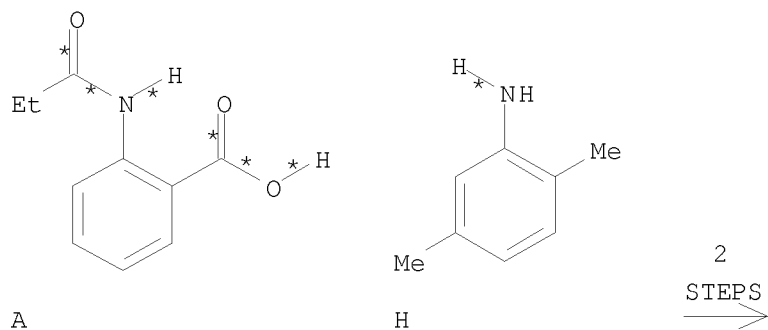
G  
YIELD 25%

RX(1)        RCT    A 19165-26-5  
              PRO    B 2916-09-8  
              CAT    75-07-0 MeCHO

RX(3)        RCT    B 2916-09-8, F 89-62-3  
              PRO    G 85731-87-9

RX(12) OF 17 COMPOSED OF RX(1), RX(4)  
RX(12)       A    +    H    ==>    I

10/ 562,112

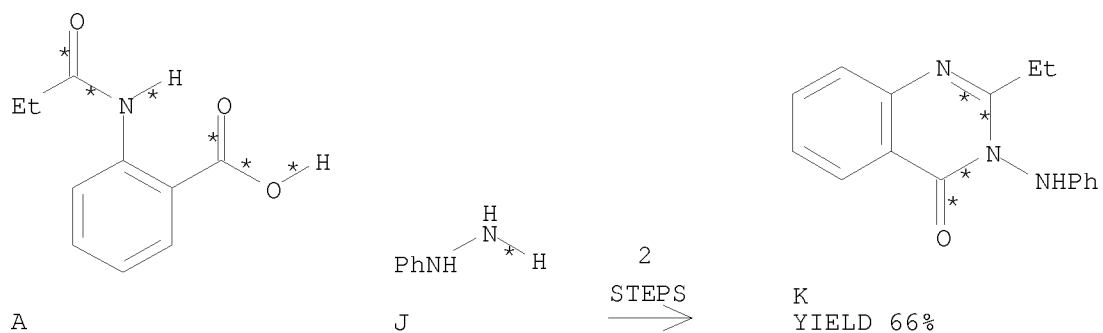


I  
YIELD 37%

RX(1) RCT A 19165-26-5  
PRO B 2916-09-8  
CAT 75-07-0 MeCHO

RX(4) RCT B 2916-09-8, H 95-78-3  
PRO I 85731-88-0

RX(13) OF 17 COMPOSED OF RX(1), RX(5)  
RX(13) A + J ==> K



RX(1) RCT A 19165-26-5  
PRO B 2916-09-8

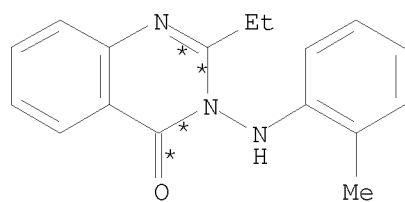
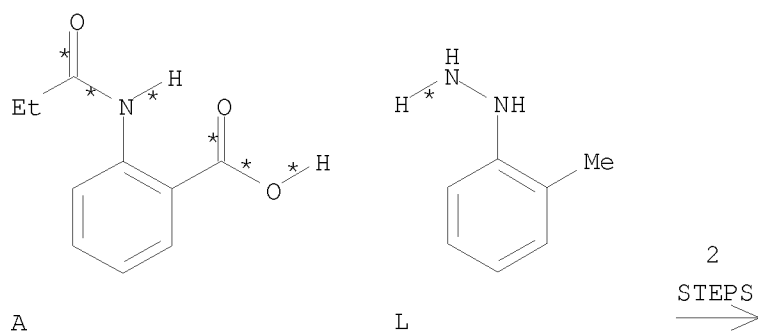
10/ 562,112

CAT 75-07-0 MeCHO

RX(5) RCT B 2916-09-8, J 100-63-0  
PRO K 50547-52-9

RX(14) OF 17 COMPOSED OF RX(1), RX(6)

RX(14) A + L ==> M



M  
YIELD 75%

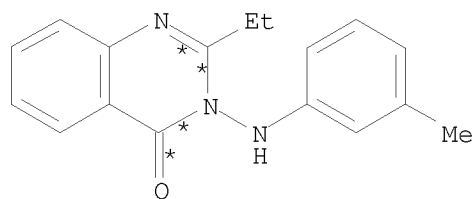
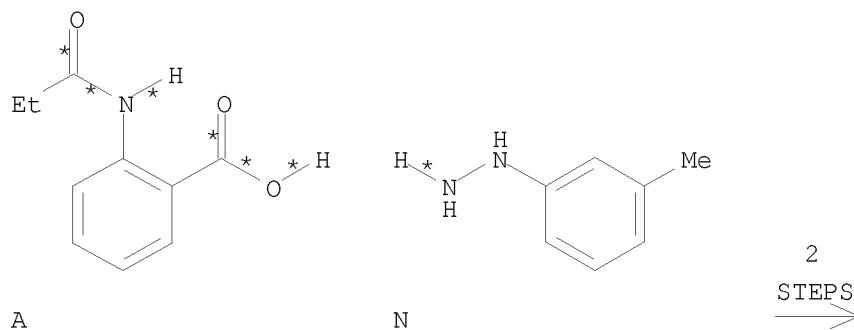
RX(1) RCT A 19165-26-5  
PRO B 2916-09-8  
CAT 75-07-0 MeCHO

RX(6) RCT B 2916-09-8, L 529-27-1  
PRO M 85731-89-1

RX(15) OF 17 COMPOSED OF RX(1), RX(7)

RX(15) A + N ==> O

10/ 562,112

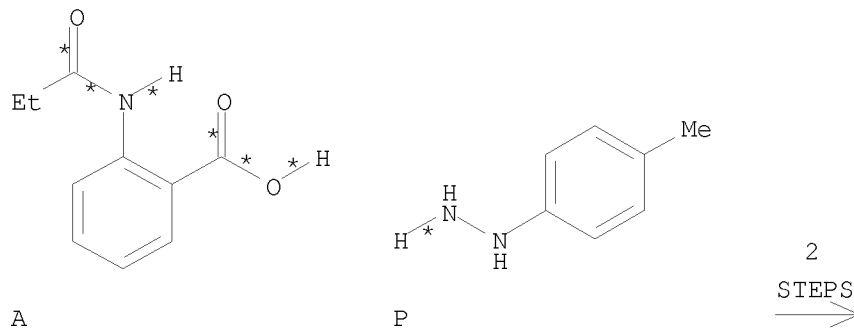


O  
YIELD 40%

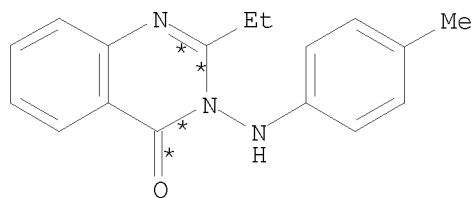
RX(1)      RCT    A 19165-26-5  
             PRO    B 2916-09-8  
             CAT    75-07-0 MeCHO

RX(7)      RCT    B 2916-09-8, N 536-89-0  
             PRO    O 85731-90-4

RX(16) OF 17 COMPOSED OF RX(1), RX(8)  
RX(16)      A    +    P    ==>    Q



10/ 562,112

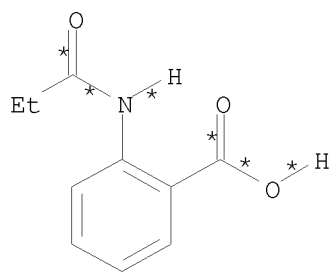


Q  
YIELD 43%

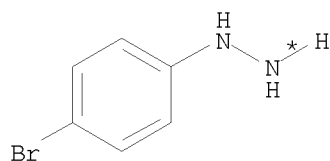
RX(1)      RCT    A 19165-26-5  
             PRO    B 2916-09-8  
             CAT    75-07-0 MeCHO

RX(8)      RCT    B 2916-09-8, P 539-44-6  
             PRO    Q 85731-91-5

RX(17) OF 17 COMPOSED OF RX(1), RX(9)  
RX(17)      A    +    R    ==>    S

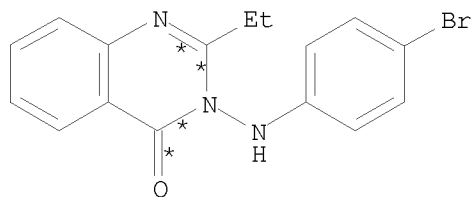


A



R

2  
STEPS  
→



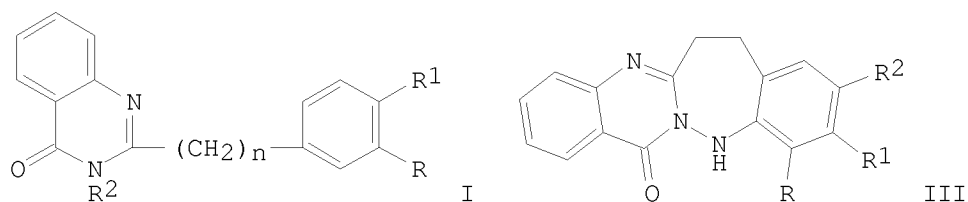
S  
YIELD 44%

RX(1)      RCT    A 19165-26-5  
             PRO    B 2916-09-8  
             CAT    75-07-0 MeCHO

RX(9)      RCT    B 2916-09-8, R 589-21-9

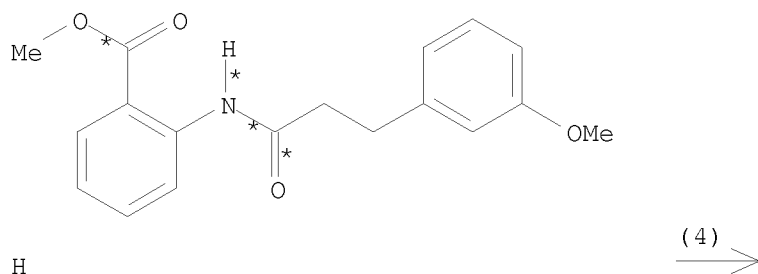
PRO S 85731-92-6

L3 ANSWER 210 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 98:16656 CASREACT  
 TITLE: Intramolecular reactions of N-nitrenes: oxidation of  
 3-amino-2-(arylalkyl)quinazolin-4(3H)-ones  
 AUTHOR(S): Atkinson, Robert S.; Malpass, John R.; Woodthorpe,  
 Katherine L.  
 CORPORATE SOURCE: Dep. Chem., Univ. Leicester, Leicester, LE1 7RH, UK  
 SOURCE: Journal of the Chemical Society, Perkin Transactions  
 1: Organic and Bio-Organic Chemistry (1972-1999)  
 (1982), (10), 2407-12  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



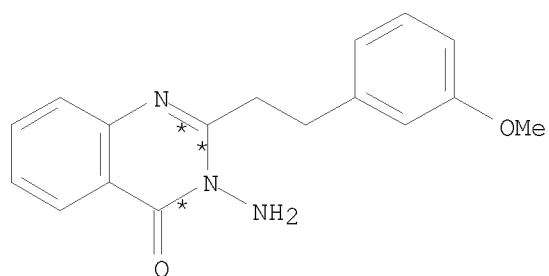
AB Oxidation of quinazolines I ( $R = \text{OMe}$ ;  $R_1 = \text{H}$ ,  $\text{OMe}$ ;  $R_2 = \text{NH}_2$ ;  $n = 2$ ) with  $\text{Pd}(\text{OAc})_4$  in  $\text{CH}_2\text{Cl}_2$  at room temperature gave I (same  $R$ ,  $R_1$ ,  $n$ ;  $R_2 = \text{H}$ ) (II) and the diazepines III ( $R = \text{H}$ ,  $\text{OMe}$ ;  $R_1 \neq R_2 = \text{H}$ ,  $\text{OMe}$ ) via the corresponding N-nitrene intermediates. On oxidation under analogous conditions I ( $n = 2$ ,  $R = \text{H}$ ,  $R_1 = \text{OMe}$ ;  $n = 1$ ,  $R \neq R_1 = \text{H}$ ,  $\text{OMe}$ ;  $R_2 = \text{NH}_2$ ) gave only the deamination products II. Azepine formation involves electrophilic aromatic substitution by the nitrene on the aromatic ring via a 7-membered transition state.

RX(4) OF 38 ...H ==> I...





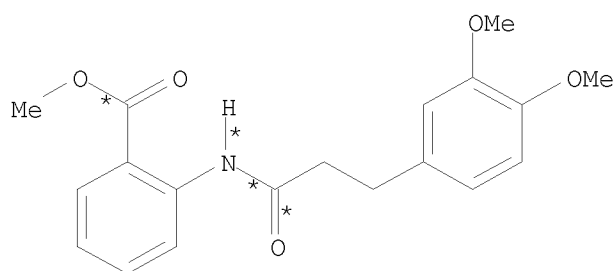
10/ 562,112



I

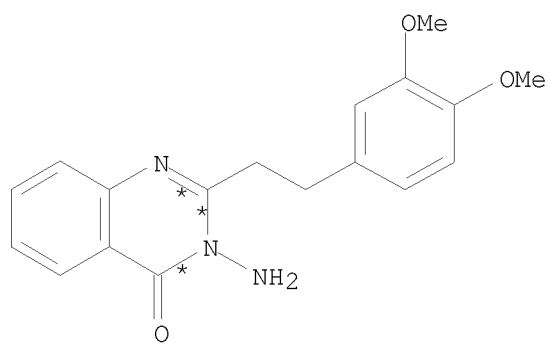
RX(4)      RCT   H 83988-42-5  
             RGT   J 302-01-2 N<sub>2</sub>H<sub>4</sub>  
             PRO   I 78649-10-2  
             SOL   67-56-1 MeOH

RX(5) OF 38      ...L ==> M



L

(5) 



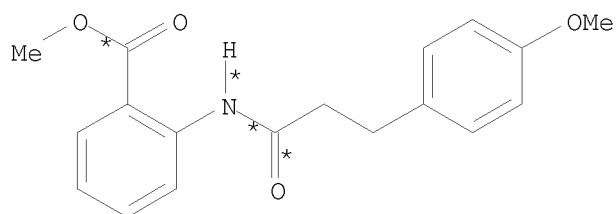
M

RX(5)      RCT   L 59282-10-9  
             RGT   J 302-01-2 N<sub>2</sub>H<sub>4</sub>

10/ 562,112

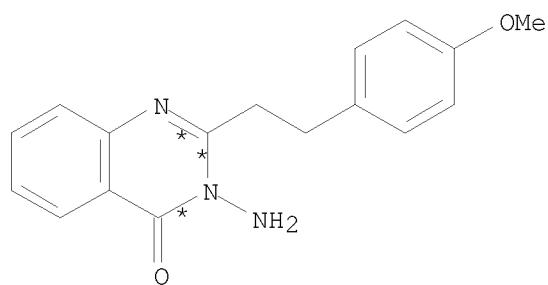
PRO M 78649-11-3  
SOL 67-56-1 MeOH

RX(6) OF 38 ...N ==> O...



N

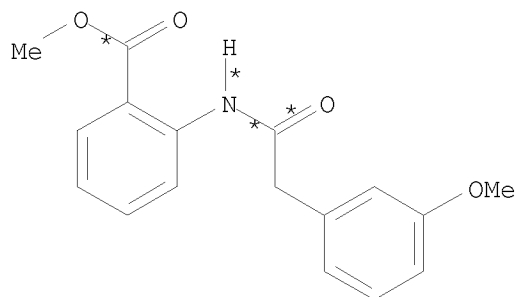
(6)  $\longrightarrow$



O

RX(6) RCT N 83988-43-6  
RGT J 302-01-2 N2H4  
PRO O 78649-12-4  
SOL 67-56-1 MeOH

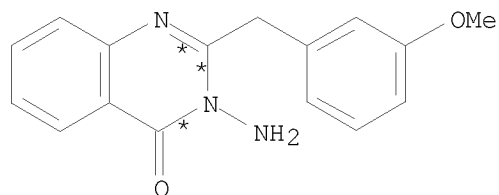
RX(7) OF 38 ...P ==> Q



P

(7)  $\longrightarrow$

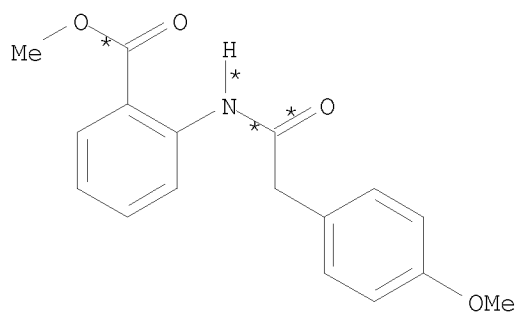
10/ 562,112



Q

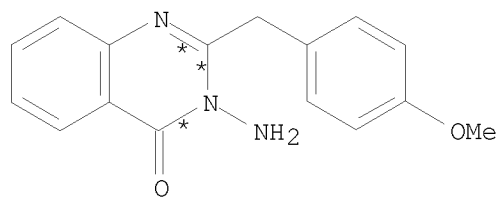
RX(7)      RCT    P 83988-44-7  
             RGT    J 302-01-2 N2H4  
             PRO    Q 83988-47-0  
             SOL    67-56-1 MeOH

RX(8) OF 38      ...R ==> S



R

(8)  $\Rightarrow$

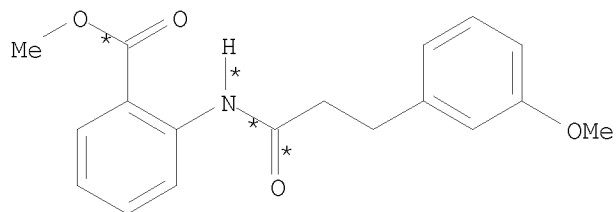


S

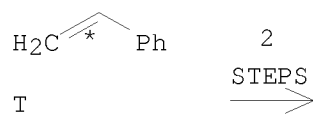
RX(8)      RCT    R 83988-45-8  
             RGT    J 302-01-2 N2H4  
             PRO    S 83988-46-9  
             SOL    67-56-1 MeOH

RX(21) OF 38 COMPOSED OF RX(4), RX(9)  
RX(21)      H    +    T    ==>    U

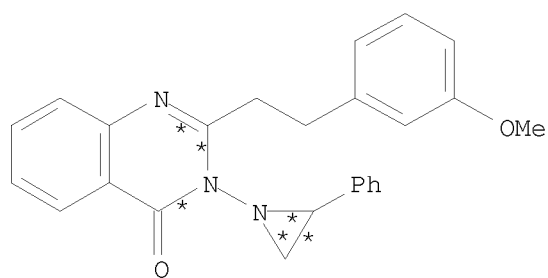
10/ 562,112



H



T

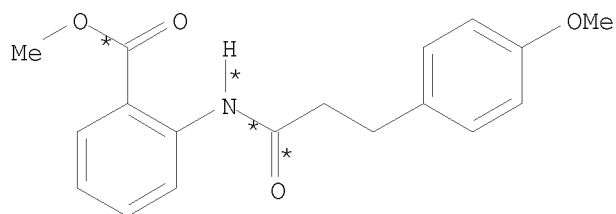


U

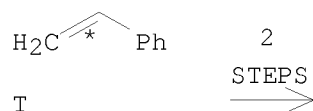
RX(4)      RCT    H 83988-42-5  
              RGT    J 302-01-2 N2H4  
              PRO    I 78649-10-2  
              SOL    67-56-1 MeOH

RX(9)      RCT    I 78649-10-2, T 100-42-5  
              PRO    U 78649-18-0  
              SOL    75-09-2 CH2Cl2

RX(22) OF 38 COMPOSED OF RX(6), RX(10)  
 RX(22)      N    +    T    ==>    W

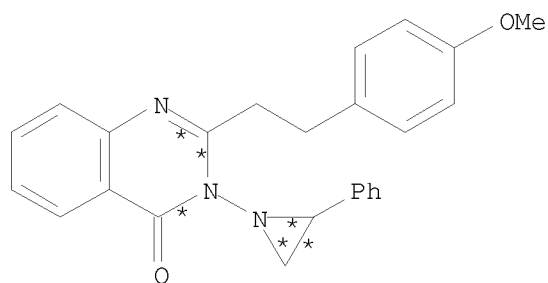


N



T

10/ 562,112

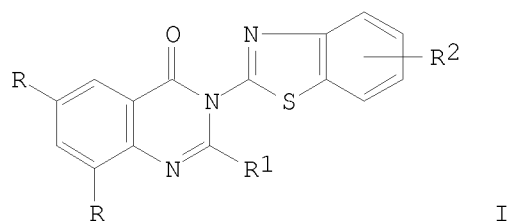


W

RX(6) RCT N 83988-43-6  
RGT J 302-01-2 N2H4  
PRO O 78649-12-4  
SOL 67-56-1 MeOH

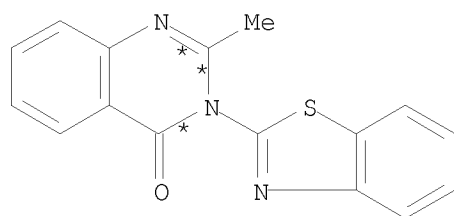
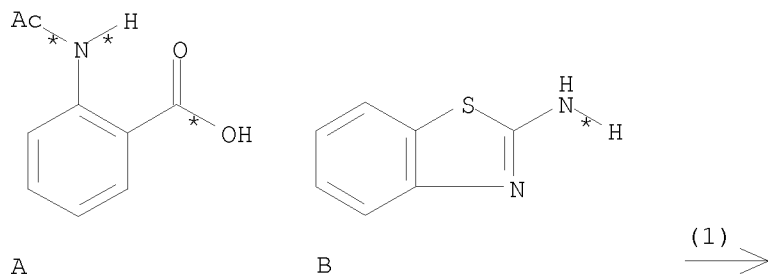
RX(10) RCT O 78649-12-4, T 100-42-5  
PRO W 78649-19-1  
SOL 75-09-2 CH2Cl2

L3 ANSWER 211 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 97:72319 CASREACT  
TITLE: Synthesis of some new 4(3H)-quinazolinones as  
potential CNS depressants  
AUTHOR(S): Chaurasia, M. Ram; Sharma, Surendra K.  
CORPORATE SOURCE: Dep. Chem., D.A.V.(P.G.) Coll., Dehra Dun, India  
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1982),  
315(4), 377-81  
CODEN: ARPMAS; ISSN: 0365-6233  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



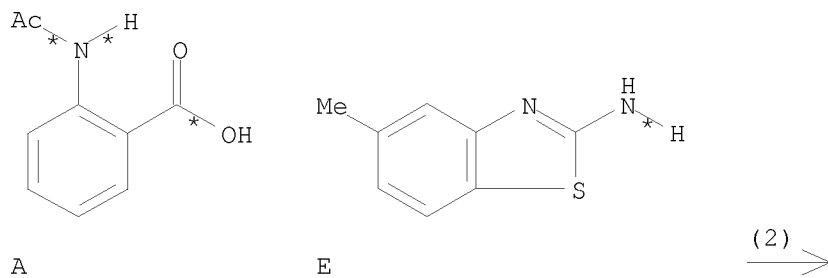
AB Quinazolinones I (R = H, Br, R1 = Me, styryl; R2 = H, Me, Cl, OMe, Et, Br in 4-, 5-, or 6-positions) were prepared by condensing the appropriate N-acetylanthranilic acid with 2-aminobenzothiazoles in the presence PCl3 (4 h in refluxing toluene) followed by optional reaction with benzaldehyde. Five I were tested for CNS depressant activity in mice and found to be active.

RX(1) OF 34      A + B ==&gt; C

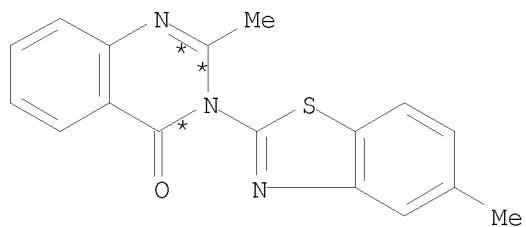
C  
YIELD 51%

RX(1)      RCT    A 89-52-1, B 136-95-8  
              RGT    D 7719-12-2 PC13  
              PRO    C 81762-52-9

RX(2) OF 34      A + E ==&gt; F



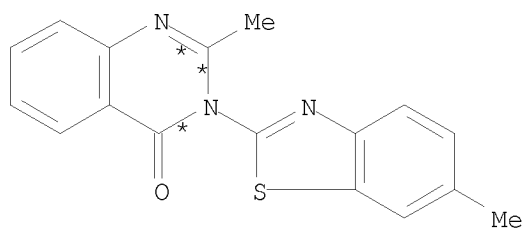
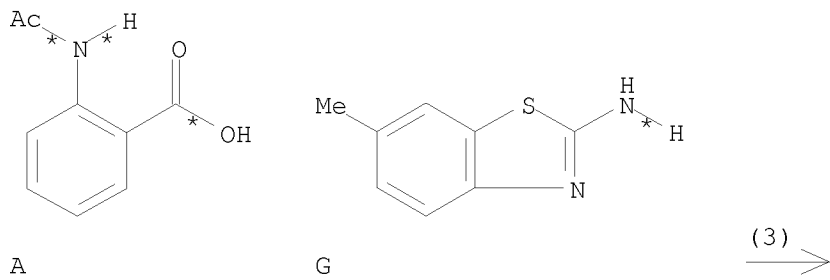
10/ 562,112



F  
YIELD 45%

RX(2)      RCT    A 89-52-1, E 14779-17-0  
             RGT    D 7719-12-2 PC13  
             PRO    F 81762-54-1

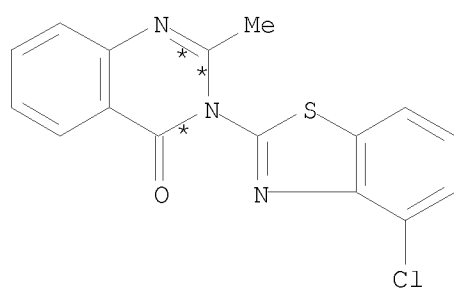
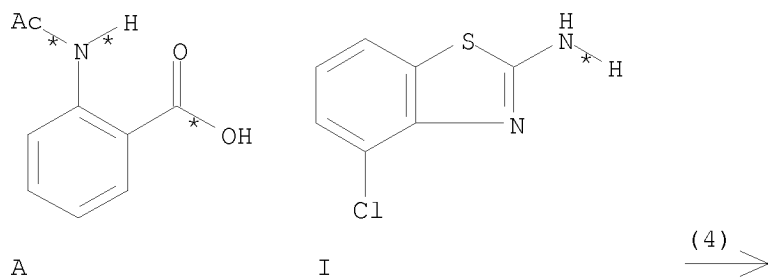
RX(3) OF 34                    A + G ==> H



H  
YIELD 49%

RX(3)            RCT    A 89-52-1, G 2536-91-6  
                  RGT    D 7719-12-2 PC13  
                  PRO    H 81762-55-2

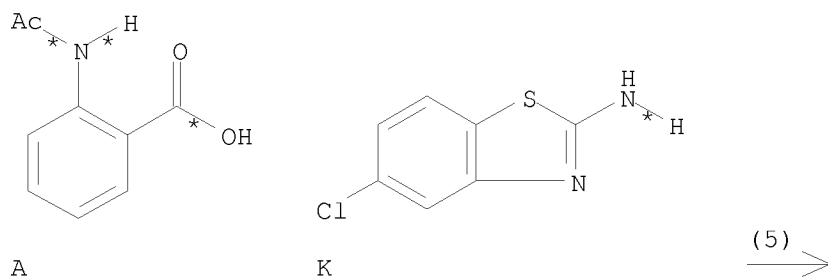
RX (4) OF 34                    A   +   I   ==>   J



YIELD 35%

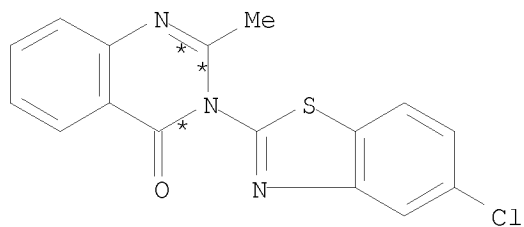
RX(4) RCT A 89-52-1, I 19952-47-7  
 RGT D 7719-12-2 PC13  
 PRO J 81762-56-3

RX(5) OF 34 A + K  $\implies$  L





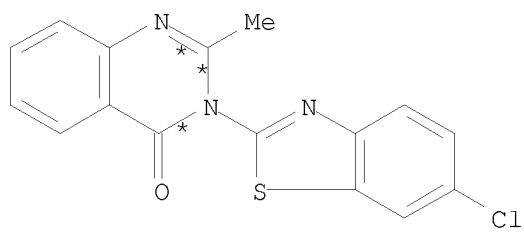
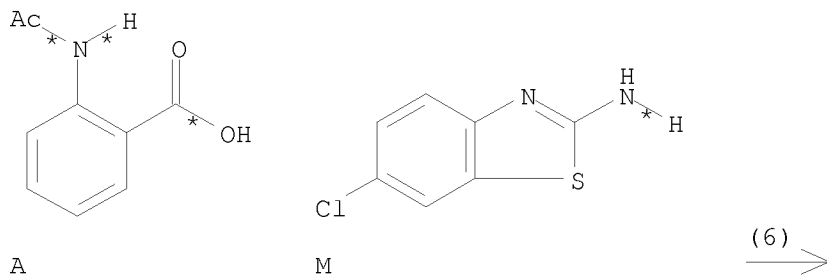
10/ 562,112



L  
YIELD 48%

RX(5)      RCT   A 89-52-1, K 20358-00-3  
              RGT   D 7719-12-2 PC13  
              PRO   L 81762-57-4

RX(6) OF 34            A   +   M   ==>   N...

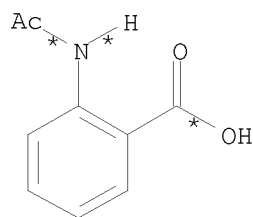


N  
YIELD 36%

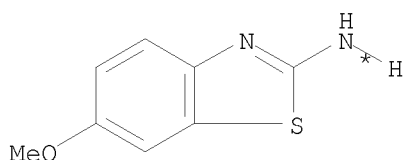
RX(6)        RCT    A 89-52-1, M 95-24-9  
              RGT    D 7719-12-2 PC13  
              PRO    N 81762-58-5

RX (7) OF 34                    A   +   O   ==>   P

10/ 562,112

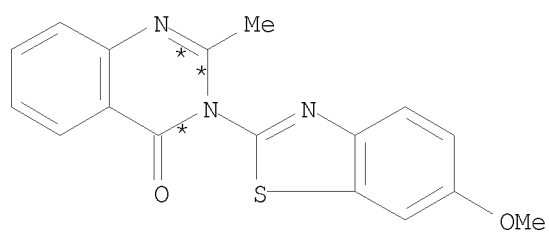


A



O

(7)  $\longrightarrow$

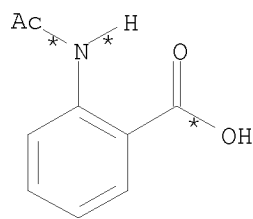


P

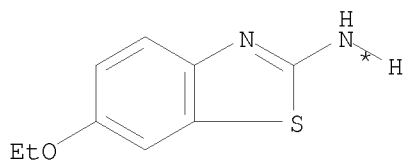
YIELD 32%

RX(7)      RCT    A 89-52-1, O 1747-60-0  
              RGT    D 7719-12-2 PC13  
              PRO    P 81762-60-9

RX(8) OF 34      A + Q  $\implies$  R...



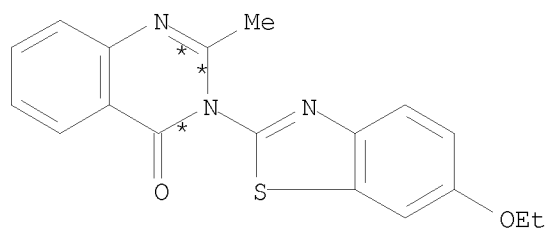
A



Q

(8)  $\longrightarrow$

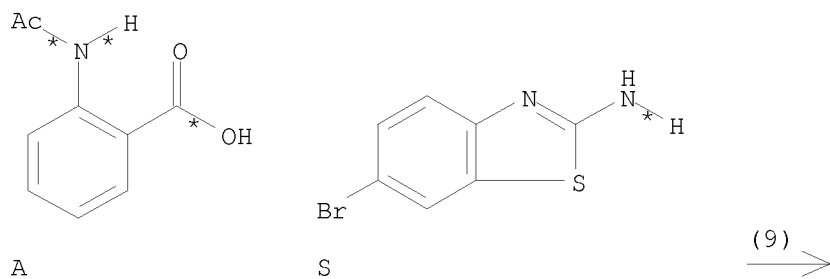
10/ 562,112



R  
YIELD 74%

RX(8) RCT A 89-52-1, Q 94-45-1  
RGT D 7719-12-2 PC13  
PRO R 81762-61-0

RX(9) OF 34 A + S ==> T

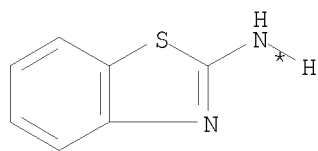


T  
YIELD 52%

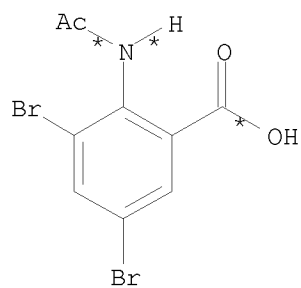
RX(9) RCT A 89-52-1, S 15864-32-1  
RGT D 7719-12-2 PC13  
PRO T 81797-04-8

RX(10) OF 34 B + U ==> V

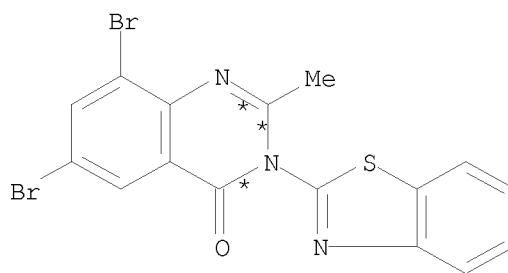
10/ 562,112



B



U

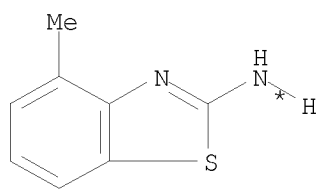


V  
YIELD 60%

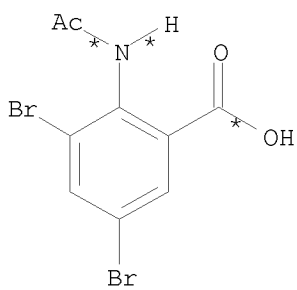
(10)

RX(10)      RCT   B 136-95-8, U 16610-45-0  
               RGT   D 7719-12-2 PC13  
               PRO   V 81762-62-1

RX(11) OF 34      W + U ==> X



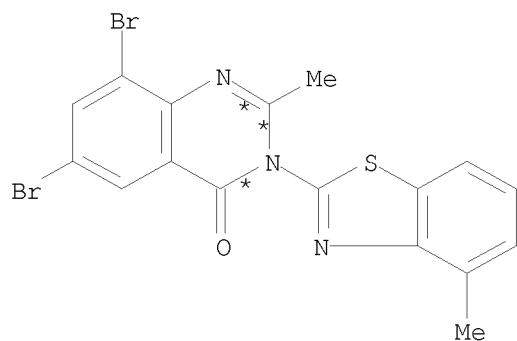
W



U

(11)

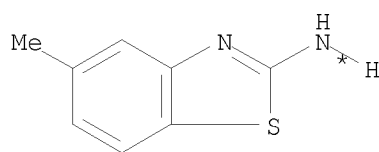
10/ 562,112



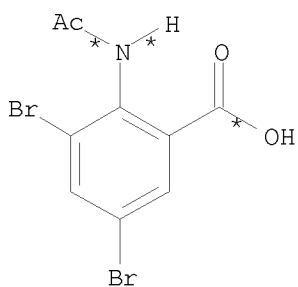
X  
YIELD 42%

RX(11) RCT W 1477-42-5, U 16610-45-0  
RGT D 7719-12-2 PC13  
PRO X 81762-63-2

RX(12) OF 34 E + U ==> Y

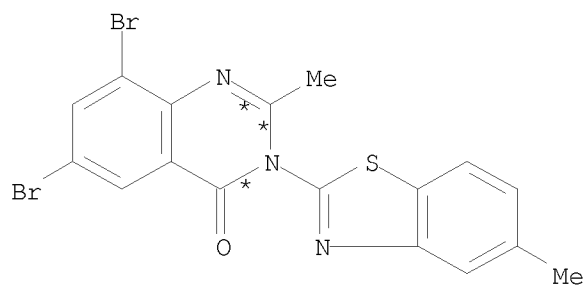


E



U

(12)  
→



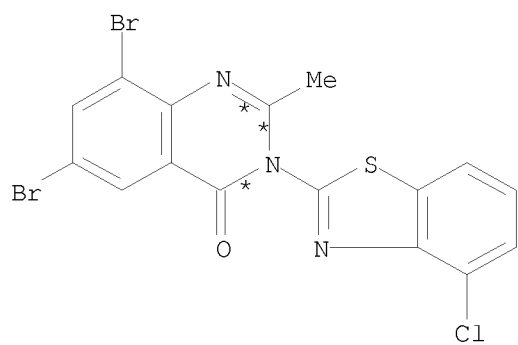
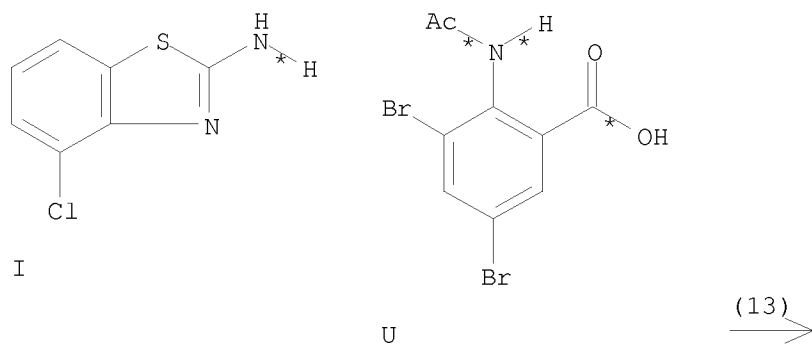
Y  
YIELD 51%

RX(12) RCT E 14779-17-0, U 16610-45-0

10/ 562,112

PRO Y 81762-64-3

RX(13) OF 34 I + U ==> Z

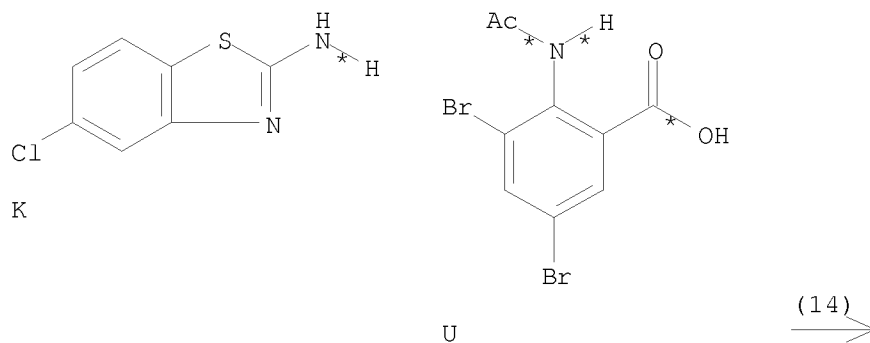


Z  
YIELD 58%

RX(13) RCT I 19952-47-7, U 16610-45-0  
RGT D 7719-12-2 PC13  
PRO Z 81762-66-5

RX(14) OF 34 K + U ==> AA

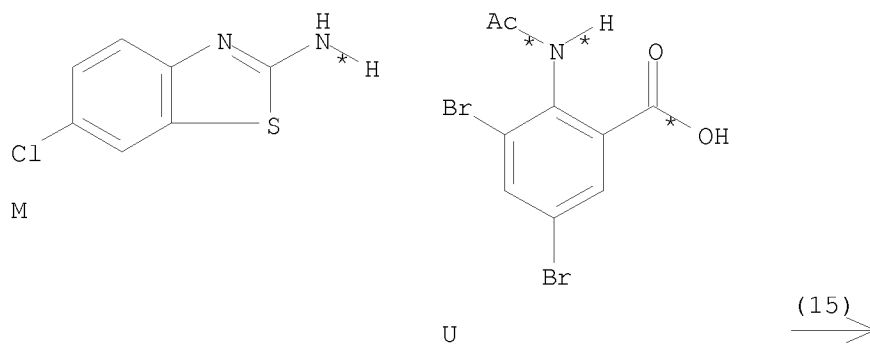
10/ 562,112



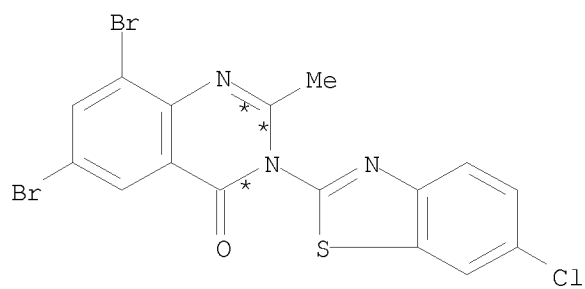
AA  
YIELD 62%

RX(14) RCT K 20358-00-3, U 16610-45-0  
RGT D 7719-12-2 PC13  
PRO AA 81762-67-6

RX(15) OF 34 M + U ==> AB...



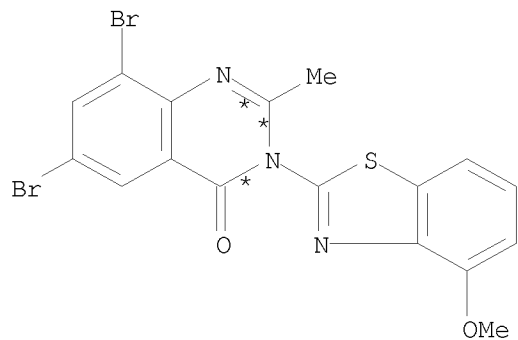
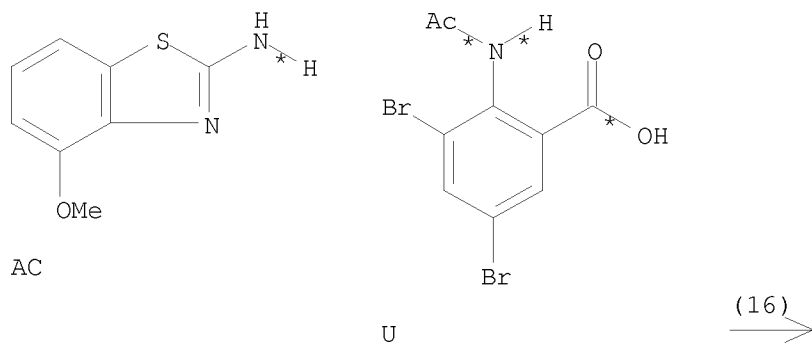
10/ 562,112



AB  
YIELD 49%

RX(15)      RCT    M 95-24-9, U 16610-45-0  
              RGT    D 7719-12-2 PC13  
              PRO    AB 81762-68-7

RX(16) OF 34      AC    +    U    ==>    AD...



AD  
YIELD 46%

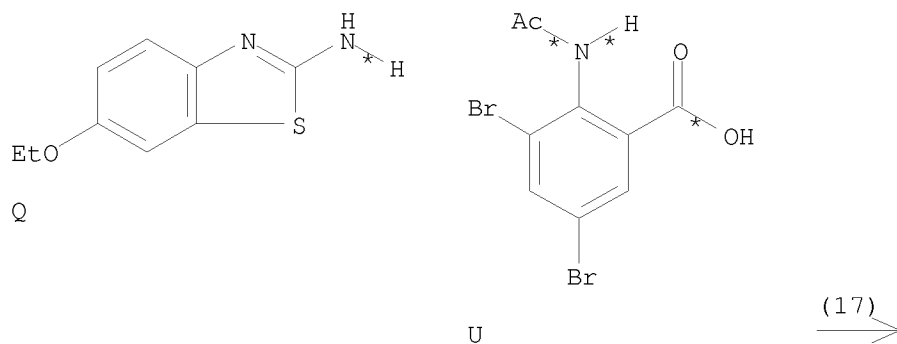
RX(16)      RCT    AC 5464-79-9, U 16610-45-0



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RGT D 7719-12-2 PC13  
PRO AD 81762-69-8

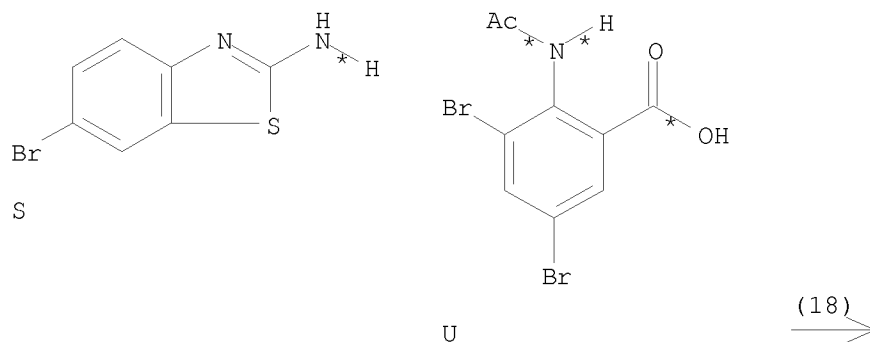
RX(17) OF 34 Q + U ==> AE



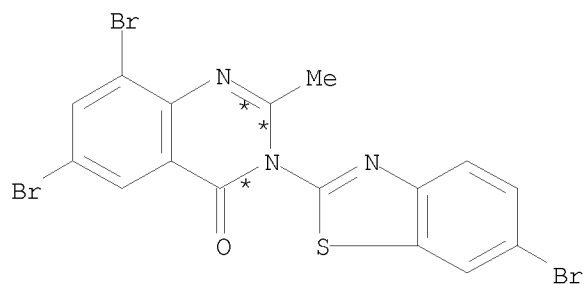
AE  
YIELD 61%

RX(17) RCT Q 94-45-1, U 16610-45-0  
RGT D 7719-12-2 PC13  
PRO AE 81762-71-2

RX(18) OF 34 S + U ==> AF



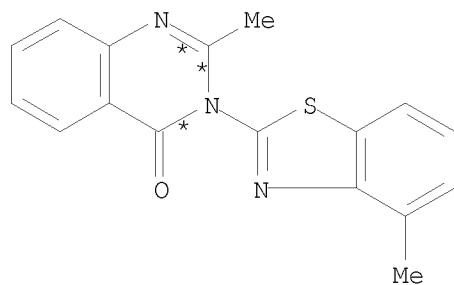
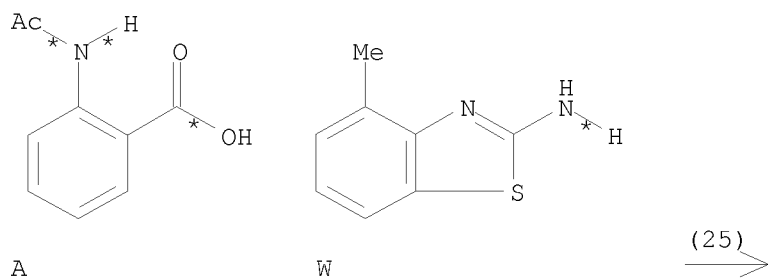
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AF  
YIELD 59%

RX(18) RCT S 15864-32-1, U 16610-45-0  
RGT D 7719-12-2 PC13  
PRO AF 81762-72-3

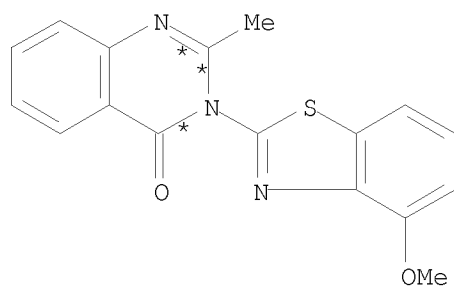
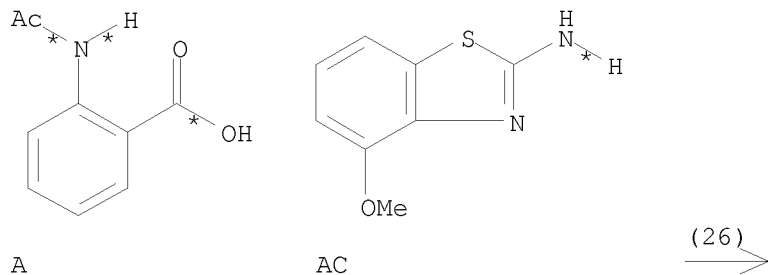
RX(25) OF 34 A + W ==> AG...



AG  
YIELD 55%

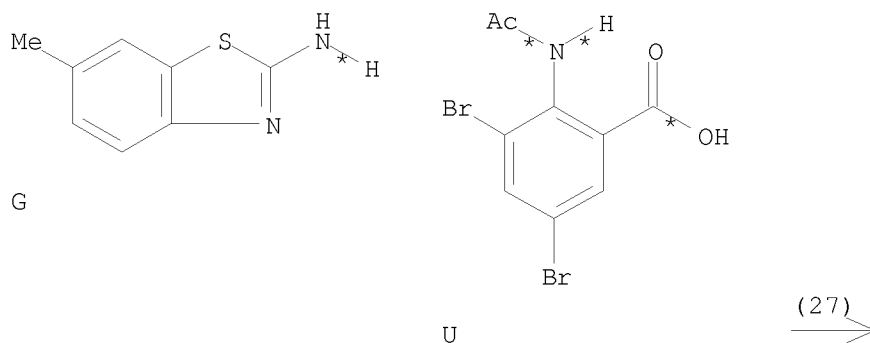
RX(25) RCT A 89-52-1, W 1477-42-5  
RGT D 7719-12-2 PC13  
PRO AG 81762-53-0

RX(26) OF 34      A + AC ==&gt; AP

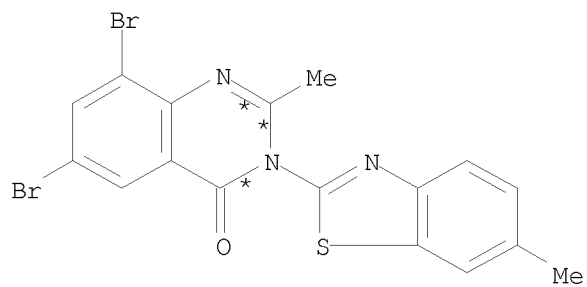
AP  
YIELD 31%

RX(26)      RCT    A 89-52-1, AC 5464-79-9  
               RGT    D 7719-12-2 PC13  
               PRO    AP 81762-59-6

RX(27) OF 34      G + U ==&gt; AL...



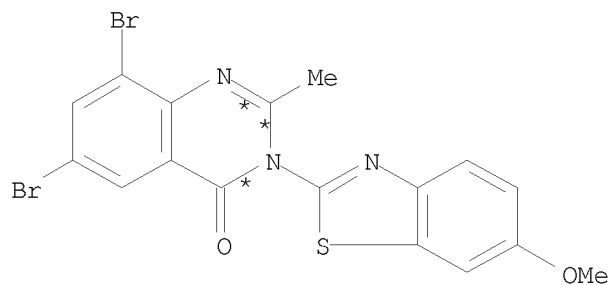
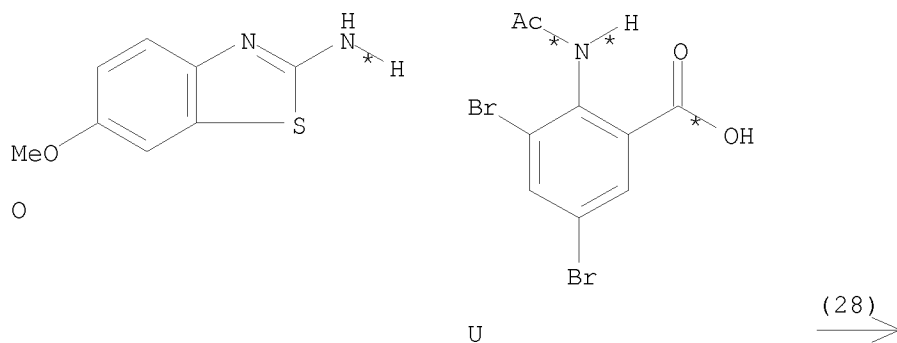
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AL  
YIELD 52%

RX(27)      RCT   G 2536-91-6, U 16610-45-0  
             RGT   D 7719-12-2 PC13  
             PRO   AL 81762-65-4

RX(28) OF 34      O   +   U   ==>   AQ

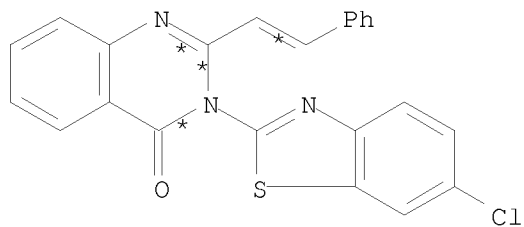
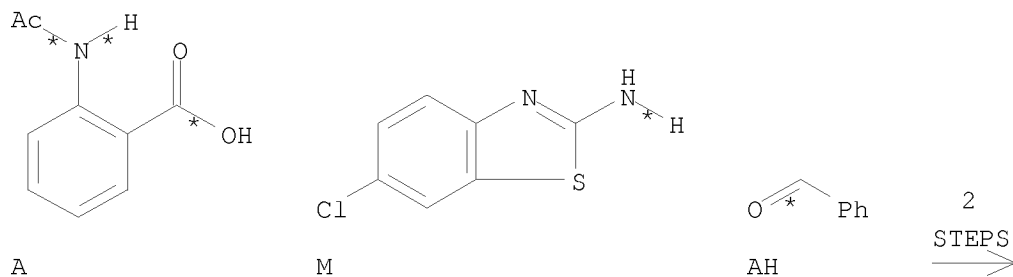


AQ  
YIELD 56%

RX(28)      RCT   O 1747-60-0, U 16610-45-0  
             RGT   D 7719-12-2 PC13  
             PRO   AQ 81762-70-1

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RX(29) OF 34 COMPOSED OF RX(6), RX(20)  
RX(29) A + M + AH ==> AJ

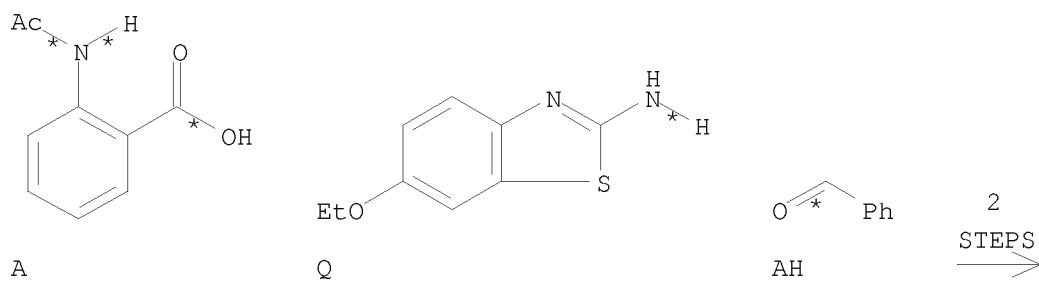


AJ  
YIELD 65%

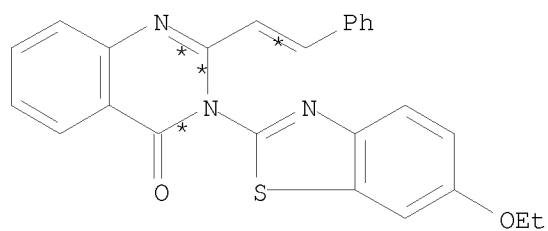
RX(6) RCT A 89-52-1, M 95-24-9  
RGT D 7719-12-2 PC13  
PRO N 81762-58-5

RX(20) RCT N 81762-58-5, AH 100-52-7  
PRO AJ 344572-35-6

RX(30) OF 34 COMPOSED OF RX(8), RX(21)  
RX(30) A + Q + AH ==> AK



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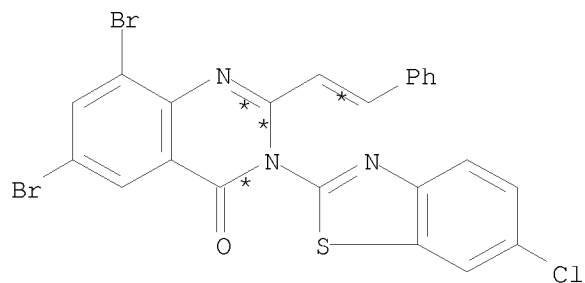
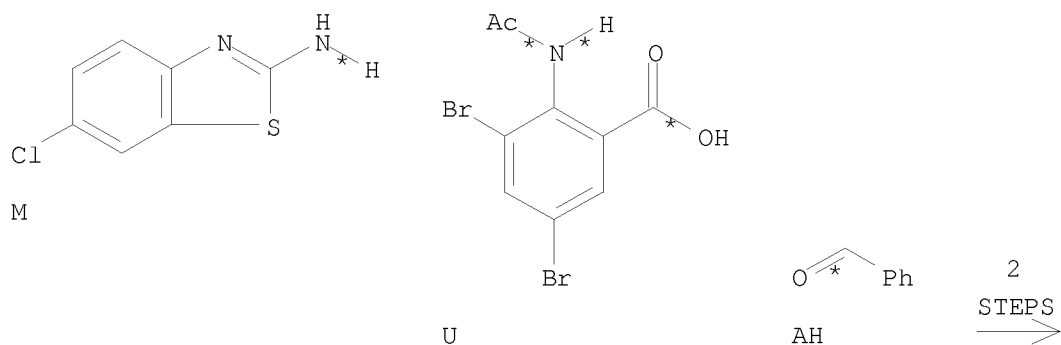


AK  
YIELD 61%

RX(8) RCT A 89-52-1, Q 94-45-1  
RGT D 7719-12-2 PC13  
PRO R 81762-61-0

RX(21) RCT R 81762-61-0, AH 100-52-7  
PRO AK 344586-30-7

RX(31) OF 34 COMPOSED OF RX(15), RX(23)  
RX(31) M + U + AH ==> AN



AN  
YIELD 69%

RX(15) RCT M 95-24-9, U 16610-45-0  
RGT D 7719-12-2 PC13

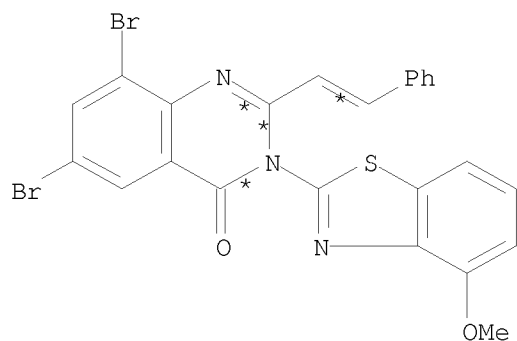
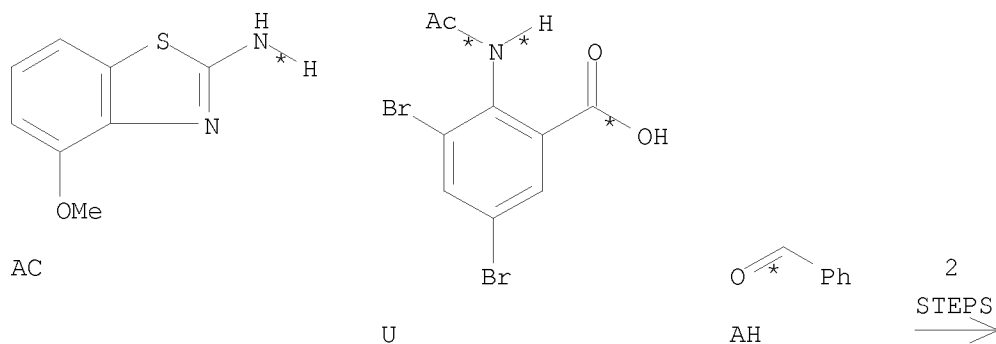
10/ 562,112

PRO AB 81762-68-7

RX(23) RCT AB 81762-68-7, AH 100-52-7  
PRO AN 344586-29-4

RX(32) OF 34 COMPOSED OF RX(16), RX(24)

RX(32) AC + U + AH ==> AO



AO  
YIELD 49%

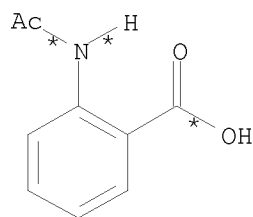
RX(16) RCT AC 5464-79-9, U 16610-45-0  
RGT D 7719-12-2 PC13  
PRO AD 81762-69-8

RX(24) RCT AD 81762-69-8, AH 100-52-7  
PRO AO 344587-22-0

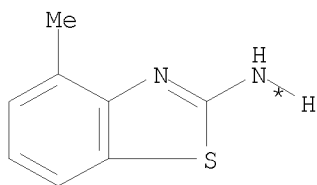
RX(33) OF 34 COMPOSED OF RX(25), RX(19)

RX(33) A + W + AH ==> AI

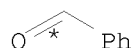
10/ 562,112



A

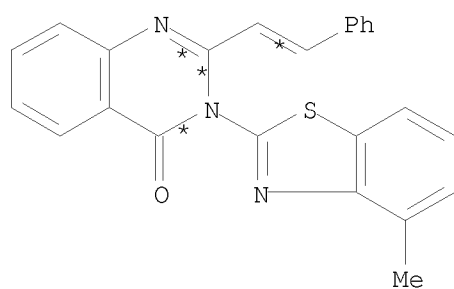


W



AH

2  
STEPS  
→

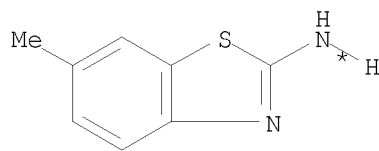


AI  
YIELD 71%

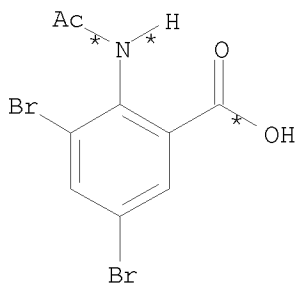
RX(25)      RCT    A 89-52-1, W 1477-42-5  
              RGT    D 7719-12-2 PC13  
              PRO    AG 81762-53-0

RX(19)      RCT    AG 81762-53-0, AH 100-52-7  
              PRO    AI 344572-36-7

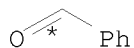
RX(34) OF 34 COMPOSED OF RX(27), RX(22)  
RX(34)      G    +    U    +    AH    ==>    AM



G



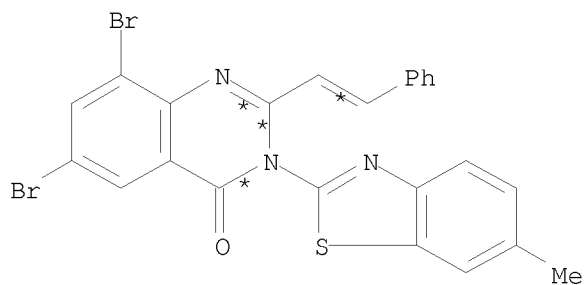
U



AH

2  
STEPS  
→



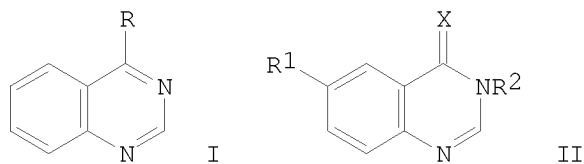


AM  
YIELD 59%

RX(27) RCT G 2536-91-6, U 16610-45-0  
RGT D 7719-12-2 PC13  
PRO AL 81762-65-4

RX(22) RCT AL 81762-65-4, AH 100-52-7  
PRO AM 344586-28-3

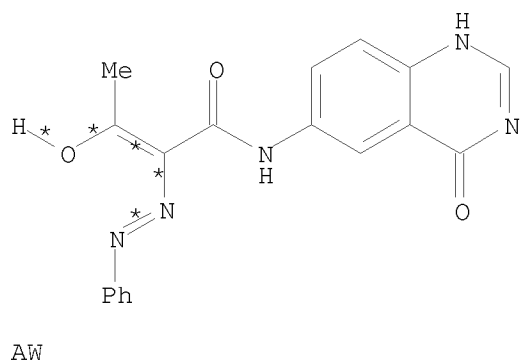
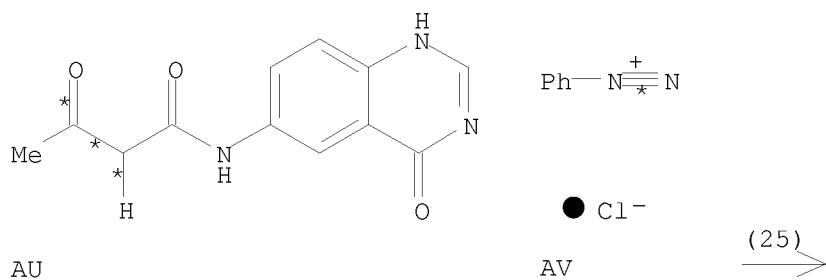
L3 ANSWER 212 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 97:55767 CASREACT  
TITLE: Some reactions of 4-chloroquinazoline, 6-nitro- and  
6-amino-4(3H)-quinazolones  
AUTHOR(S): Anwar, M.; Abdel-Hay, F. I.; Elbarbary, A. A.;  
El-Borai, M.  
CORPORATE SOURCE: Fac. Sci., Tanta Univ., Tanta, Egypt  
SOURCE: Revue Roumaine de Chimie (1981), 26(11-12), 1469-78  
CODEN: RRCHAX; ISSN: 0035-3930  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Quinazolines I [R = NHCONH<sub>2</sub>, NHCHO, NHAc, NAcPh, NAcC<sub>6</sub>H<sub>4</sub>Me-2, NAcC<sub>6</sub>H<sub>4</sub>Me-4, N-acetyl-N-1-naphthylamino, NHNHC<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>-4, NHNHC<sub>6</sub>H<sub>3</sub>(NO<sub>2</sub>)<sub>2</sub>-2,4] were prepared by aminating I (R = Cl). II (X = O, S; R<sub>1</sub> = H, NO<sub>2</sub>; R<sub>2</sub> = aminomethyl) were obtained by aminomethylating II (R<sub>2</sub> = H). II (X = O, R<sub>1</sub> = NH<sub>2</sub>, R<sub>2</sub> = H) was treated with MeCOCH<sub>2</sub>CO<sub>2</sub>Et to give II (X = O, R<sub>1</sub> = NHC(=O)CH<sub>2</sub>COMe, R<sub>2</sub> = H) which was treated with 4-R<sub>3</sub>C<sub>6</sub>H<sub>4</sub>N<sub>2</sub><sup>+</sup> (R<sub>3</sub> = H, Me, OMe) to give II [X = O, R<sub>1</sub> = 4-R<sub>3</sub>C<sub>6</sub>H<sub>4</sub>N:NC(:CMeOH)CONH, R<sub>2</sub> = H].

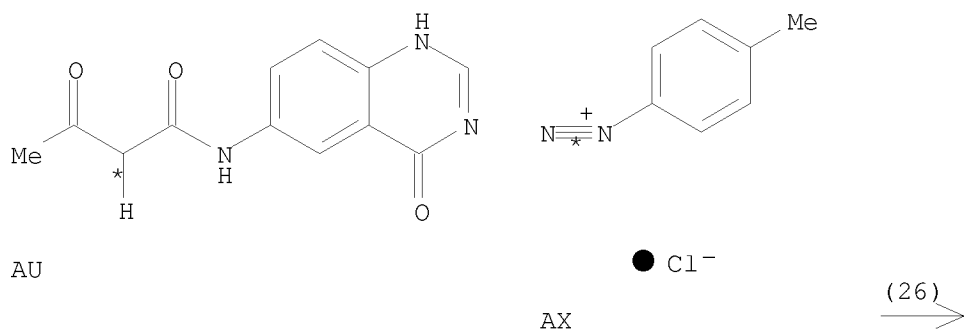
10/ 562,112

RX(25) OF 32 ...AU + AV ==> AW

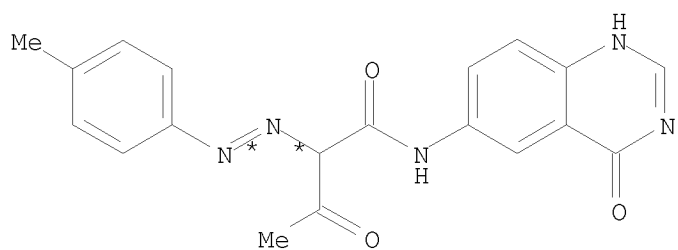


RX(25) RCT AU 40368-25-0, AV 100-34-5  
PRO AW 345627-06-7

RX(26) OF 32 ...AU + AX ==> AY



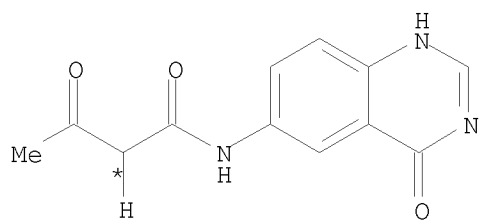
10/ 562,112



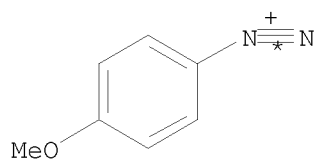
AY

RX(26) RCT AU 40368-25-0, AX 2028-84-4  
PRO AY 82436-16-6

RX(27) OF 32 ...AU + AZ ==> BA



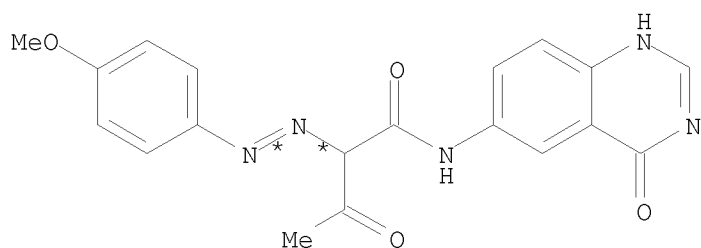
AU



AZ



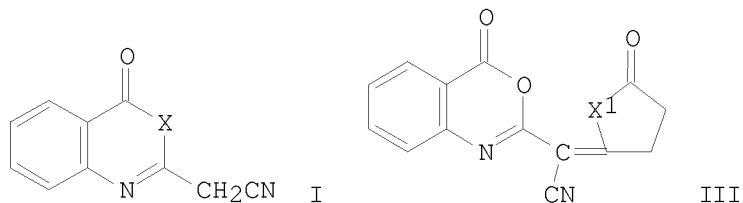
10/ 562,112



BA

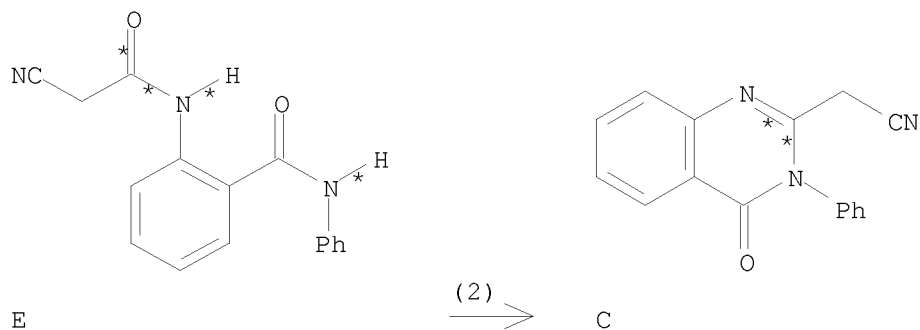
RX(27) RCT AU 40368-25-0, AZ 4346-59-2  
PRO BA 82436-17-7

L3 ANSWER 213 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 96:20043 CASREACT  
TITLE: Reactions of 2-cyanomethyl-3,1-benzoxazin-4(H)-one  
with nucleophilic reagents, acid anhydrides and acid  
imides  
AUTHOR(S): Mohamed, M. M.; El-Hashash, M. A.; Esswy, A.; Shaban,  
M. E.  
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt  
SOURCE: Indian Journal of Chemistry, Section B: Organic  
Chemistry Including Medicinal Chemistry (1981),  
20B(8), 718-19  
CODEN: IJSBDB; ISSN: 0376-4699  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



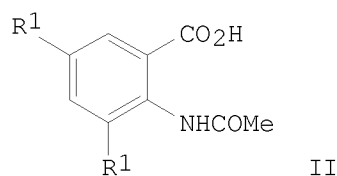
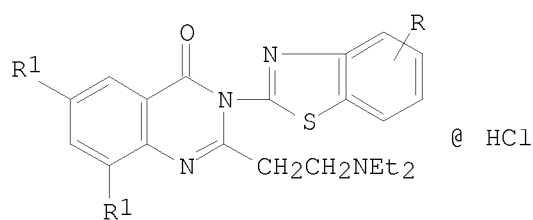
AB Refluxing benzoxazinone (I) (X = O) (II) with N<sub>2</sub>H<sub>4</sub> and PhNHNH<sub>2</sub> in EtOH  
gave I (X = NNH<sub>2</sub>, NNHPh), resp., whereas refluxing II with PhNH<sub>2</sub> in EtOH  
gave 2-PhNHCOC<sub>6</sub>H<sub>4</sub>NHCOCH<sub>2</sub>CN. Condensation of II with succinic anhydride  
and succinimide gave III (X<sub>1</sub> = O, NH), resp.

RX(2) OF 22 ...E ==> C



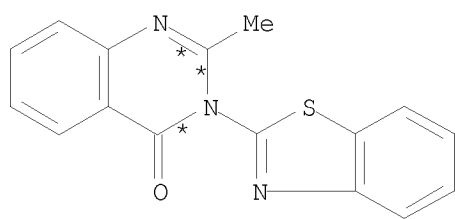
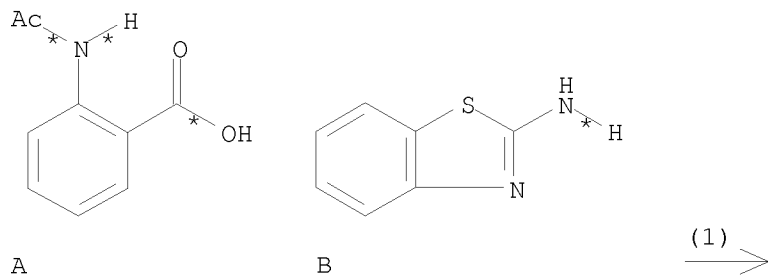
RX(2)      RCT   E 79946-29-5  
              PRO   C 20873-23-8  
              CAT   108-24-7 Ac2O

L3    ANSWER 214 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER:        96:6681    CASREACT  
 TITLE:                      Synthesis of some new 4(3H)-quinazolinones as  
                                  potential fungicides  
 AUTHOR(S):                Chaurasia, M. R.; Sharma, Surendra K.; Kumar, Sunil  
 CORPORATE SOURCE:        Dep. Chem., D.A.V. Coll., Dehra Dun, 248 001, India  
 SOURCE:                     Current Science (1981), 50(19), 841-3  
                                  CODEN: CUSCAM; ISSN: 0011-3891  
 DOCUMENT TYPE:            Journal  
 LANGUAGE:                 English  
 GI



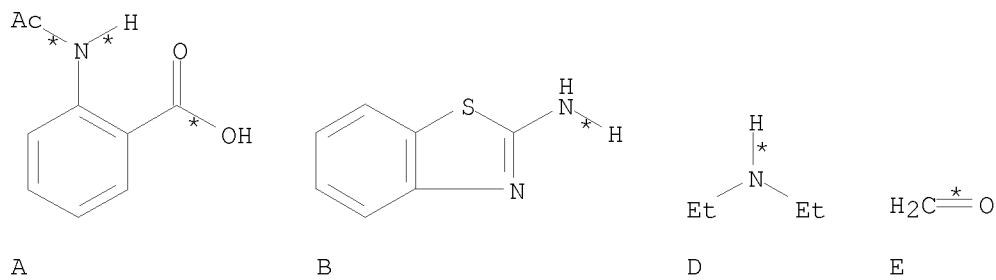
AB    Benzothiazolylquinazolines I (R = H, 4-, 5-, 6-Me, 4-, 5-, 6-Cl, 6-MeO, 6-EtO, R1 = H, Br) were prepared in 32-71% yields by cyclocondensation of II in the presence of an appropriate 2-aminobenzimidazole to give intermediates (no data) which were condensed with CH2O and Et2NH.HCl. I inhibited *Aspergillus niger* and *Draschlera australiensis*.

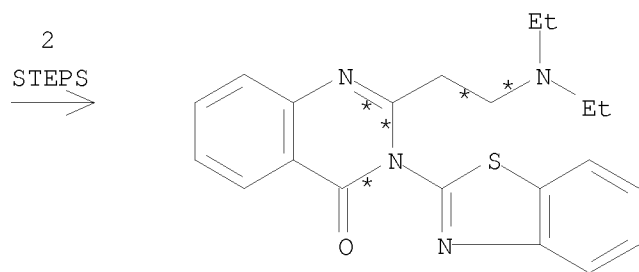
RX(1) OF 3      A + B ==> C...



RX(1)      RCT    A 89-52-1, B 136-95-8  
 PRO    C 81762-52-9

RX(3) OF 3 COMPOSED OF RX(1), RX(2)  
 RX(3)      A + B + D + E ==> F





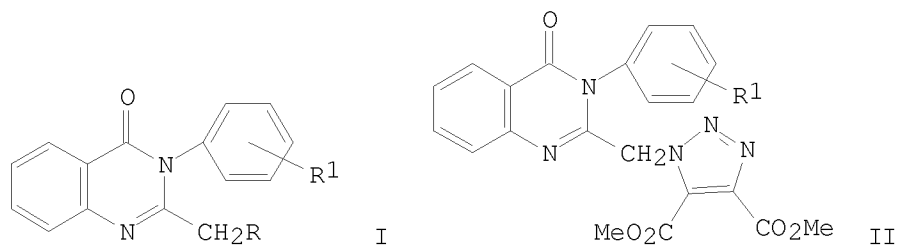
● HCl

F

RX(1) RCT A 89-52-1, B 136-95-8  
PRO C 81762-52-9

RX(2) RCT C 81762-52-9, D 109-89-7, E 50-00-0  
PRO F 80144-66-7

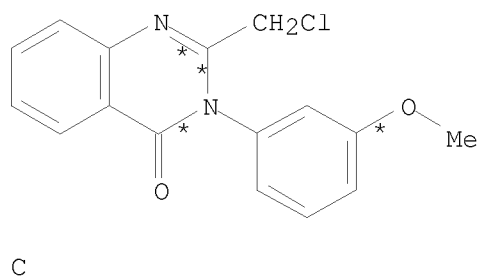
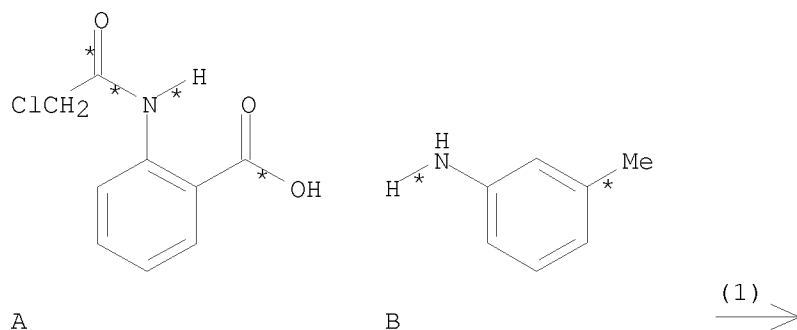
L3 ANSWER 215 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 96:6679 CASREACT  
 TITLE: Quinazolinones. 2. Syntheses and some reactions of  
 2-azidomethyl-3-aryl-4-quinazolinones  
 AUTHOR(S): Domanig, Rainer  
 CORPORATE SOURCE: Inst. Org. Pharm. Chem., Univ. Innsbruck, Innsbruck,  
 A-6020, Austria  
 SOURCE: Monatshefte fuer Chemie (1981), 112(10), 1195-202  
 CODEN: MOCMB7; ISSN: 0026-9247  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 GI



AB Starting with the chloromethyl compds. I (R = Cl; R1 = H, 2-Me, 2-MeO, 2-NO2, 3-MeO, 3,5-(MeO)2, 4-Cl, 5-NO2), the new 2-azidomethyl-3-aryl-4-quinazolinones I (R = N3) were prepared, some of which were reduced to the corresponding amines I (R = NH2) by H2S in good

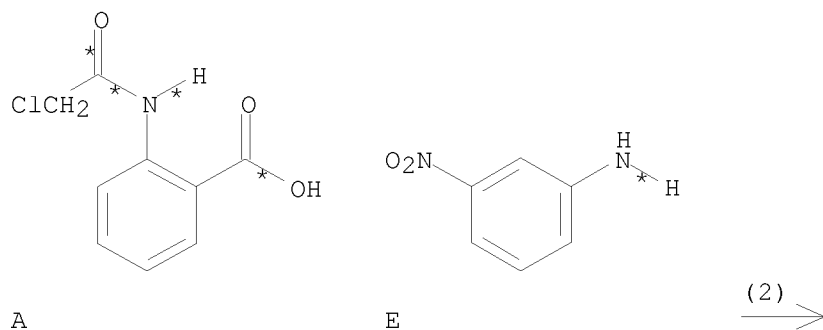
yield. As a first example of the capability of the azides to undergo 1,3-dipolar cycloaddn., II (R1 = 2-Me, 3-MeO, 4-Cl) were prepared by reacting I (R = N3) with MeO2CC.tplbond.CC(=O)OMe.

RX(1) OF 16      A + B ==> C



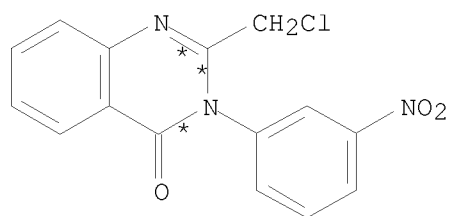
RX(1)      RCT    A 14422-49-2, B 108-44-1  
              PRO    C 76535-03-0  
              SOL    108-88-3 PhMe

RX(2) OF 16      A + E ==> F





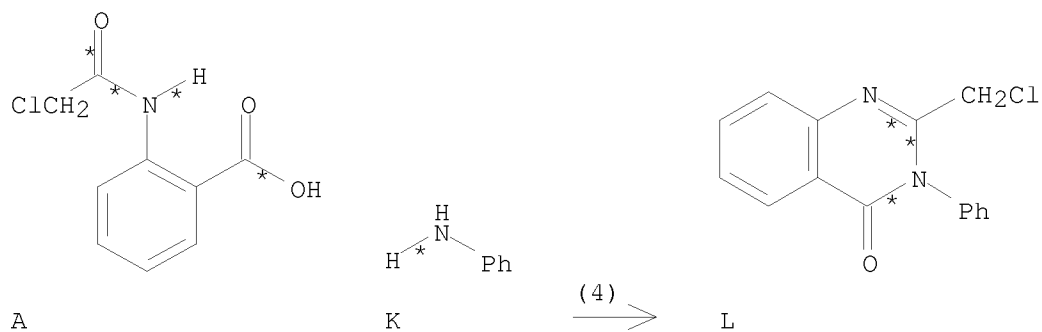
10/ 562,112



F

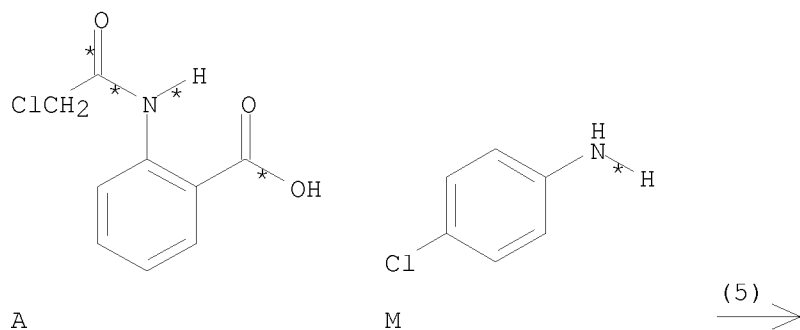
RX(2)      RCT    A 14422-49-2, E 99-09-2  
              PRO    F 80096-24-8  
              SOL    108-88-3 PhMe

RX(4) OF 16      A    +    K    ==>    L

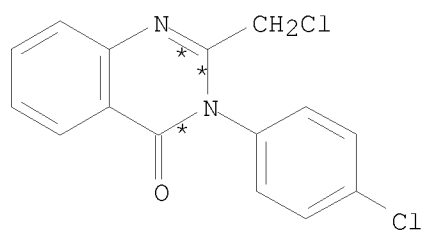


RX(4)      RCT    A 14422-49-2, K 62-53-3  
              PRO    L 22312-77-2  
              SOL    108-88-3 PhMe

RX(5) OF 16      A    +    M    ==>    N



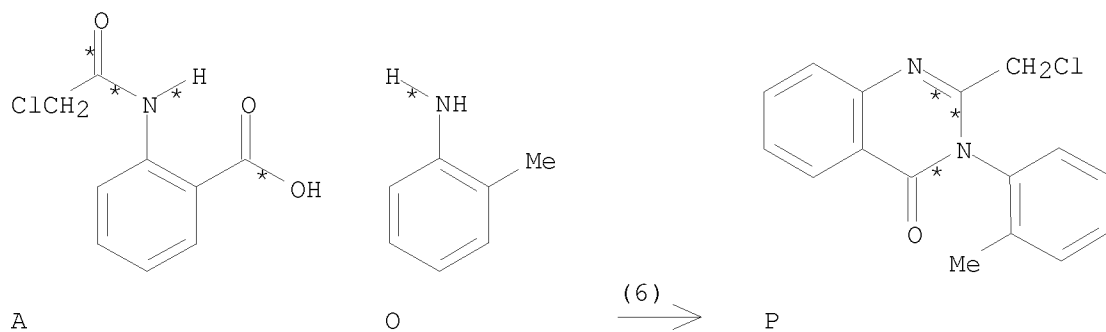
10/ 562,112



N

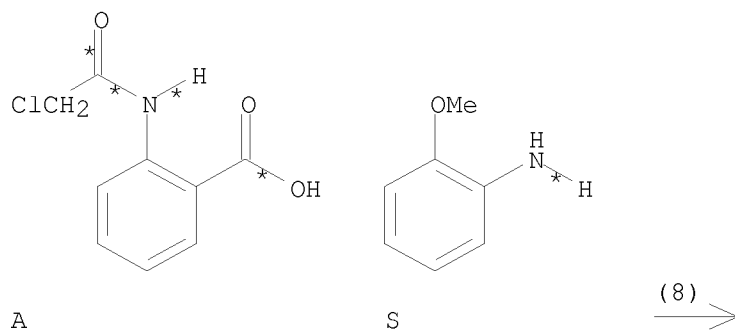
RX(5)      RCT    A 14422-49-2, M 106-47-8  
              PRO    N 22280-87-1  
              SOL    108-88-3 PhMe

RX(6) OF 16      A + O ==> P

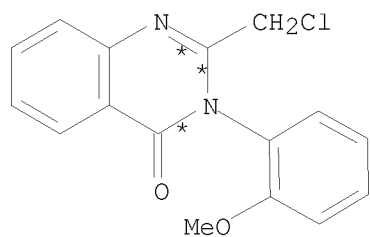


RX(6)      RCT    A 14422-49-2, O 95-53-4  
              PRO    P 3166-54-9  
              SOL    108-88-3 PhMe

RX(8) OF 16      A + S ==> T



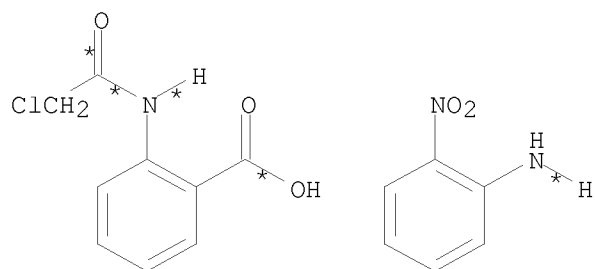
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T

RX(8)      RCT   A 14422-49-2, S 90-04-0  
              PRO   T 22312-81-8  
              SOL   108-88-3 PhMe

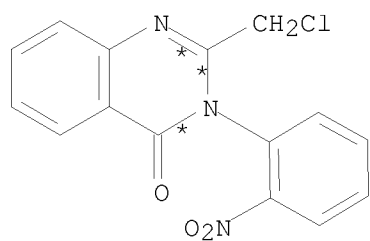
RX(9) OF 16      A   +   U   ==>   V



A

U

(9) >

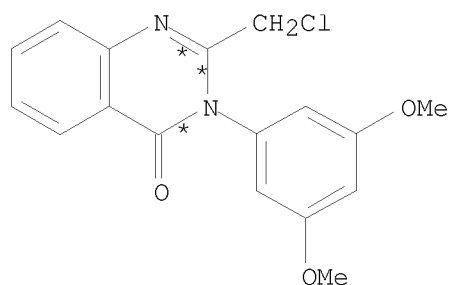
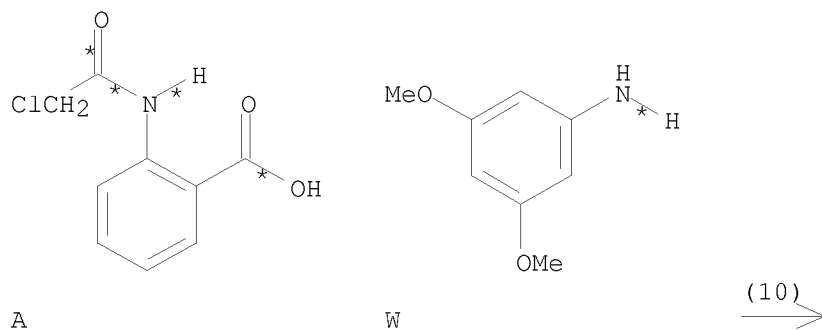


V

RX(9)      RCT   A 14422-49-2, U 88-74-4  
              PRO   V 80096-22-6  
              SOL   108-88-3 PhMe

RX(10) OF 16      A   +   W   ==>   X

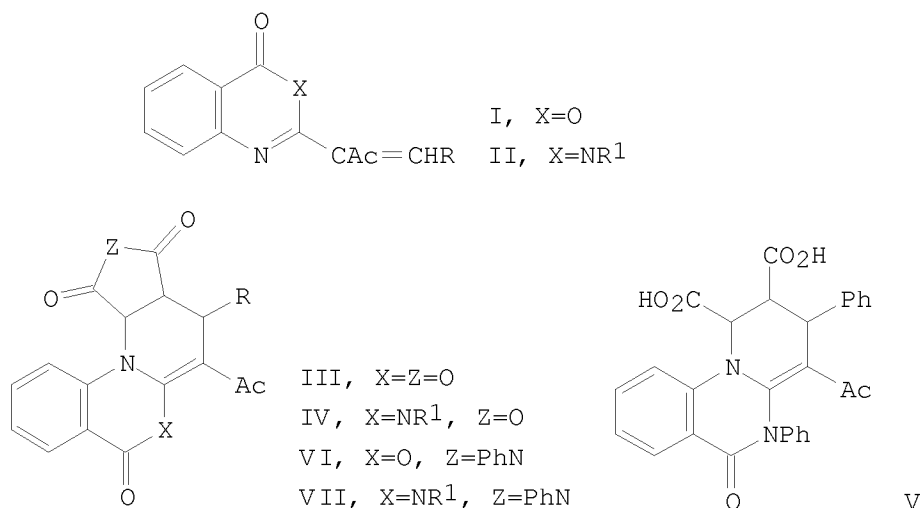
10/ 562,112



X

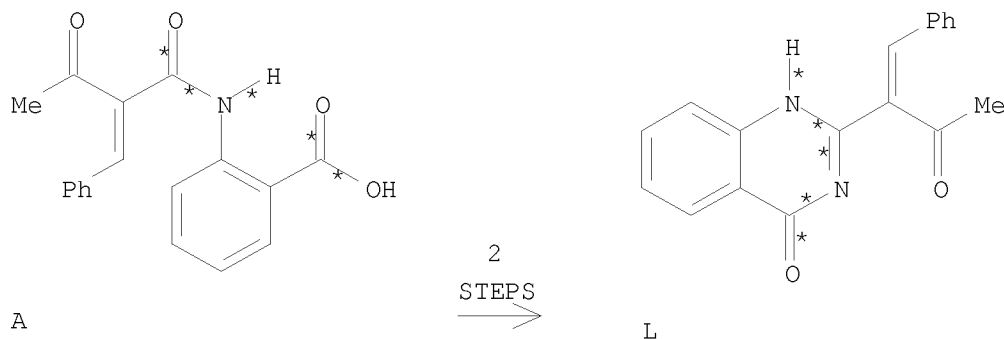
RX(10) RCT A 14422-49-2, W 10272-07-8  
PRO X 80096-23-7  
SOL 108-88-3 PhMe

L3 ANSWER 216 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 95:115443 CASREACT  
TITLE: Synthesis and reactions of  
2-( $\alpha$ -acetylstyryl)-3,1-benzoxazin-(4H)-ones and  
2-( $\alpha$ -acetylstyryl)-quinazolin-4-(3H)-ones  
AUTHOR(S): Elkasaby, M. A.; Nouredin, N. A.  
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt  
SOURCE: Indian Journal of Chemistry, Section B: Organic  
Chemistry Including Medicinal Chemistry (1981),  
20B(4), 290-3  
CODEN: IJSBDB; ISSN: 0376-4699  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Benzoxazinones I (R = Ph, p-MeOC<sub>6</sub>H<sub>4</sub>, p-Me<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>) and quinazolines II (R = Ph, p-MeOC<sub>6</sub>H<sub>4</sub>; R<sup>1</sup> = H, Ph, p-MeC<sub>6</sub>H<sub>4</sub>, p-MeOC<sub>6</sub>H<sub>4</sub>) were prepared from o-HO<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>NHCOAc:CHR. I (R = Ph, p-MeOC<sub>6</sub>H<sub>4</sub>) react with maleic anhydride to give furopyridobenzoxazines III. Several II similarly underwent Diels-Alder reaction with maleic anhydride to give the furopyridoquinazolines IV. IV (R = R<sup>1</sup> = Ph) was hydrolyzed to give the pyridoquinazoline V. II and III reacted with N-phenylmaleimide to give cycloadducts VI and VII, resp. Reaction of I with Grignard reagent and II with PhSH were investigated.

RX(35) OF 102 COMPOSED OF RX(1), RX(7)  
RX(35) A ==> L



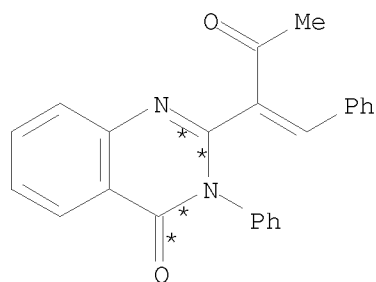
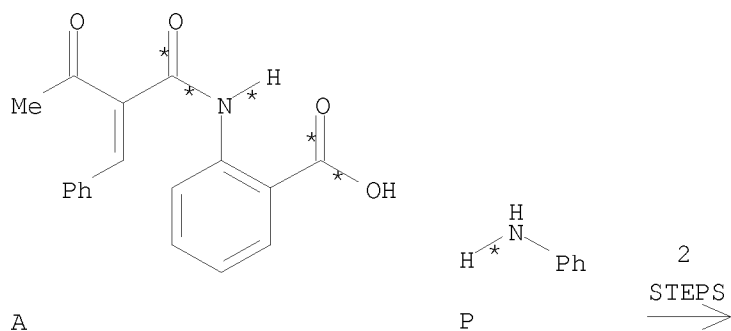
RX(1) RCT A 78817-80-8  
PRO B 70723-60-3  
CAT 108-24-7 Ac2O

RX(7) RCT B 70723-60-3  
RGT M 7664-41-7 NH<sub>3</sub>  
PRO L 78817-49-9

10/ 562,112

RX(36) OF 102 COMPOSED OF RX(1), RX(10)

RX(36)      A + P ==> Q



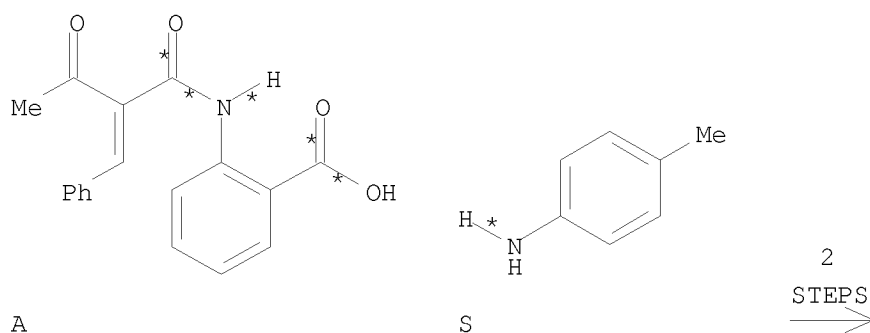
Q

RX(1)      RCT    A 78817-80-8  
             PRO    B 70723-60-3  
             CAT    108-24-7 Ac2O

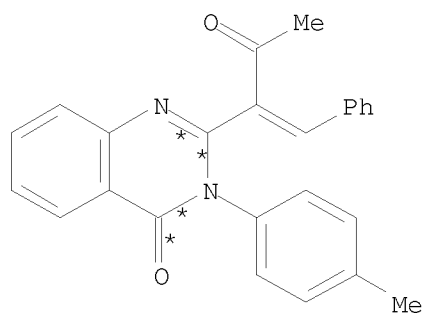
RX(10)     RCT    B 70723-60-3, P 62-53-3  
             PRO    Q 344572-47-0

RX(37) OF 102 COMPOSED OF RX(1), RX(12)

RX(37)      A + S ==> T



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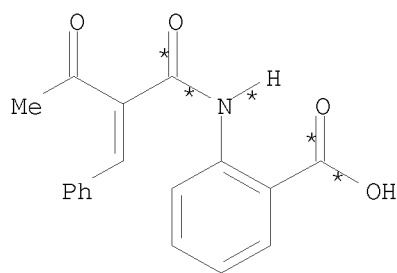


T

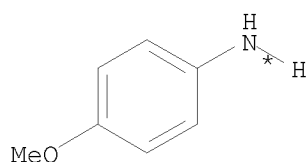
RX(1)      RCT    A 78817-80-8  
              PRO    B 70723-60-3  
              CAT    108-24-7 Ac2O

RX(12)      RCT    B 70723-60-3, S 106-49-0  
              PRO    T 344571-95-5

RX(38) OF 102 COMPOSED OF RX(1), RX(14)  
 RX(38)      A    +    V    ==>    W

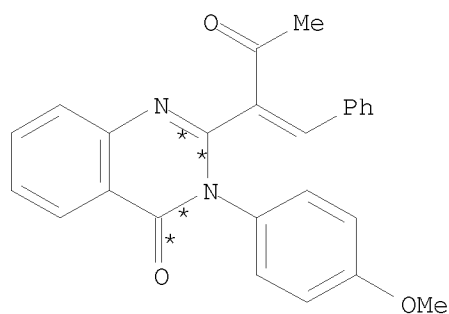


A



V

2  
 STEPS  
 —————>



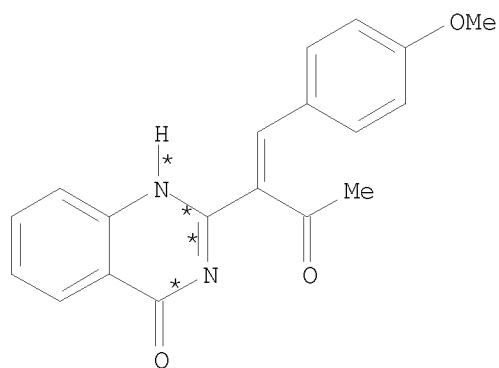
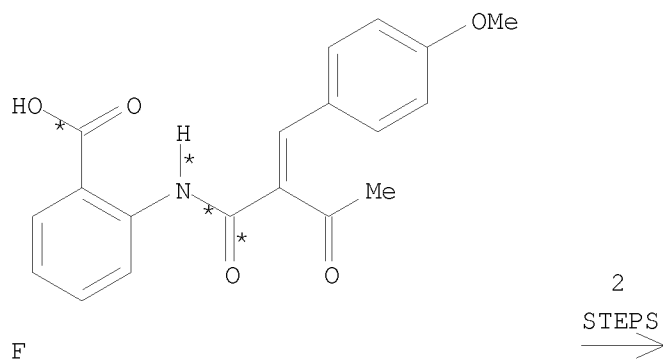
W

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RX(1)        RCT    A 78817-80-8  
              PRO    B 70723-60-3  
              CAT    108-24-7 Ac2O

RX(14)       RCT    B 70723-60-3, V 104-94-9  
              PRO    W 344580-68-3

RX(49) OF 102 COMPOSED OF RX(3), RX(8)  
RX(49)       F    ==>    N



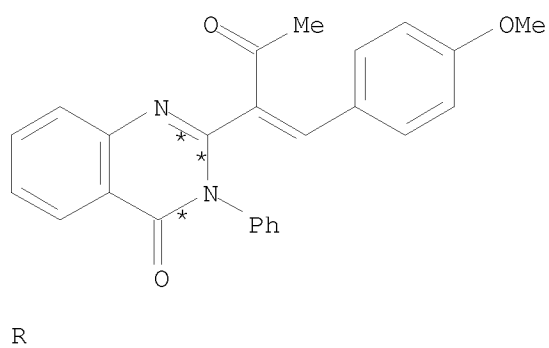
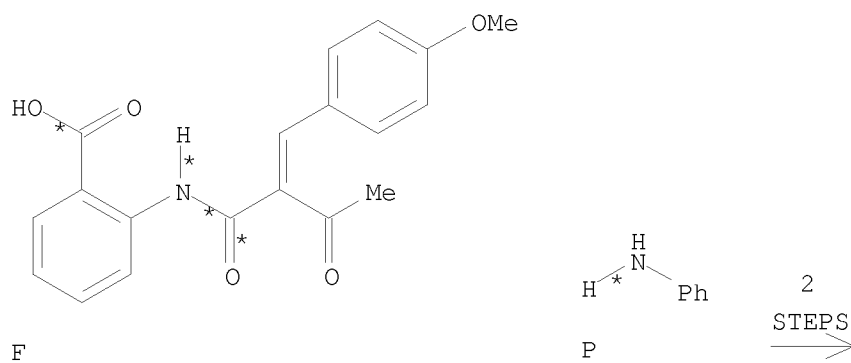
RX(3)        RCT    F 78817-81-9  
              PRO    G 70723-63-6  
              CAT    108-24-7 Ac2O

RX(8)        RCT    G 70723-63-6  
              RGT    M 7664-41-7 NH3  
              PRO    N 78817-50-2

RX(50) OF 102 COMPOSED OF RX(3), RX(11)  
RX(50)       F    +    P    ==>    R



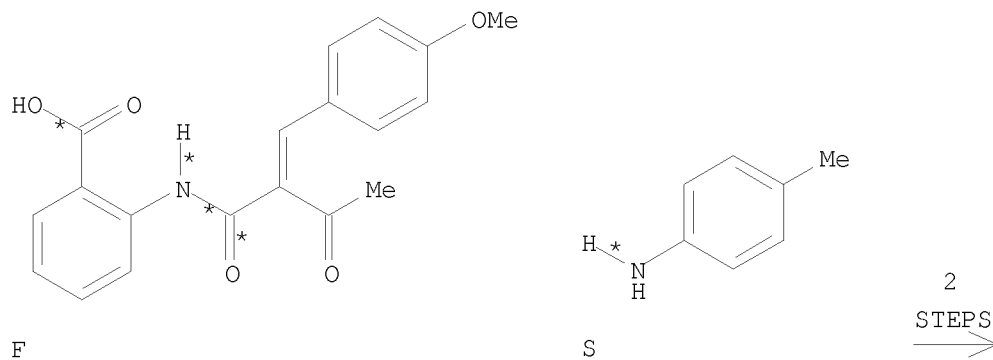
10/ 562,112



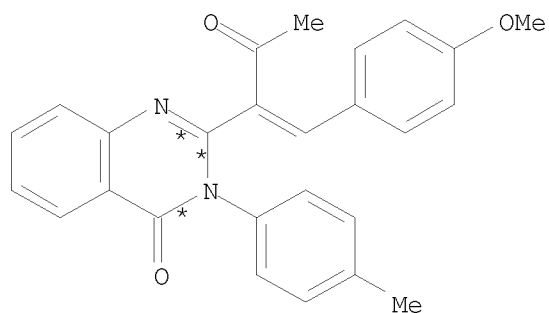
RX(3)      RCT    F 78817-81-9  
              PRO    G 70723-63-6  
              CAT    108-24-7 Ac2O

RX(11)      RCT    G 70723-63-6, P 62-53-3  
              PRO    R 344580-63-8

RX(51) OF 102 COMPOSED OF RX(3), RX(13)  
 RX(51)      F    +    S    ==>    U



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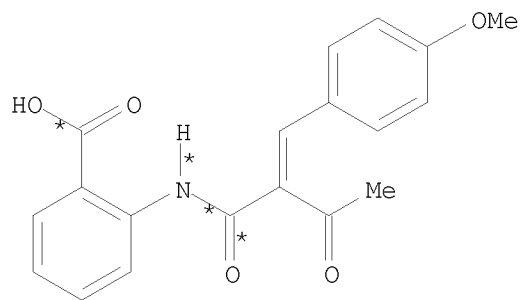


U

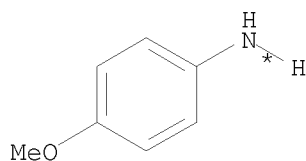
RX(3)      RCT   F 78817-81-9  
              PRO   G 70723-63-6  
              CAT   108-24-7 Ac20

RX(13)      RCT   G 70723-63-6, S 106-49-0  
              PRO   U 344581-72-2

RX(52) OF 102 COMPOSED OF RX(3), RX(15)  
 RX(52)      F   +   V   ==>   X



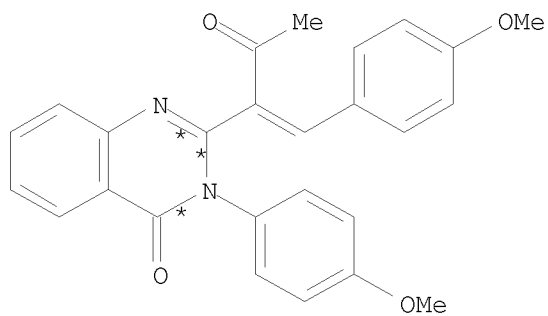
F



V

2  
 STEPS  
 →

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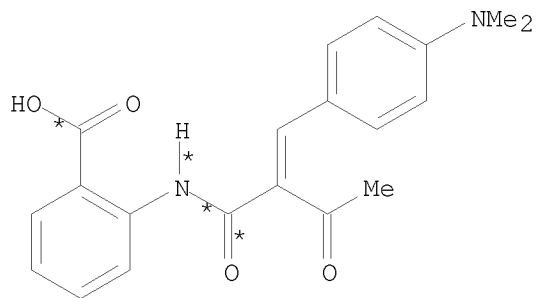


X

RX(3)      RCT   F 78817-81-9  
              PRO   G 70723-63-6  
              CAT   108-24-7   Ac2O

RX(15) RCT G 70723-63-6, V 104-94-9  
PRO X 344586-86-3

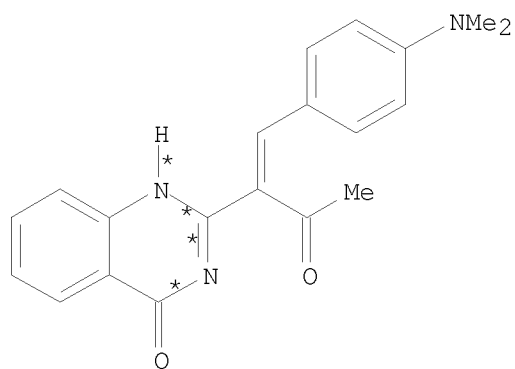
RX(59) OF 102 COMPOSED OF RX(5), RX(9)  
RX(59) I ==> 0



I

2  
STEPS

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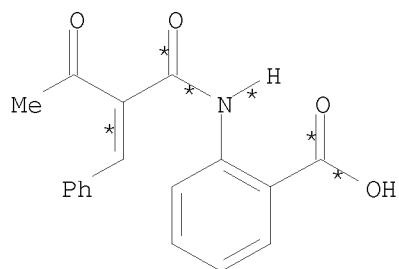


O

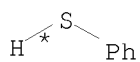
RX(5)      RCT    I 78817-82-0  
              PRO    J 78817-48-8  
              CAT    108-24-7 Ac2O

RX(9)      RCT    J 78817-48-8  
              RGT    M 7664-41-7 NH3  
              PRO    O 78922-69-7

RX(77) OF 102 COMPOSED OF RX(1), RX(7), RX(31)  
 RX(77)      A    +    AT    ==>    AU



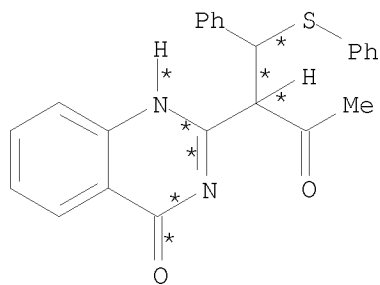
A



AT

3  
 STEPS  
 →

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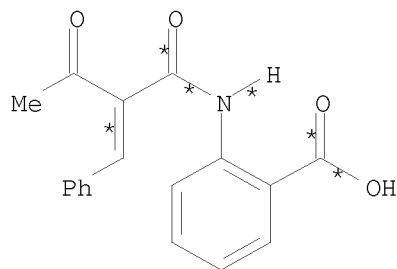
AU  
YIELD 70%

RX(1) RCT A 78817-80-8  
PRO B 70723-60-3  
CAT 108-24-7 Ac2O

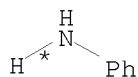
RX(7) RCT B 70723-60-3  
RGT M 7664-41-7 NH3  
PRO L 78817-49-9

RX(31) RCT L 78817-49-9, AT 108-98-5  
PRO AU 78817-76-2

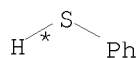
RX(81) OF 102 COMPOSED OF RX(1), RX(10), RX(32)  
RX(81) A + P + AT ==> AV



A



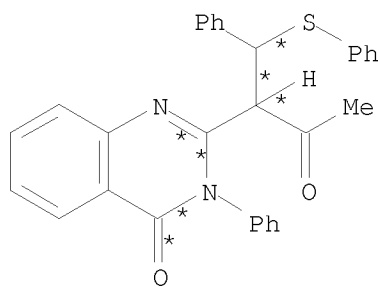
P



AT

3  
STEPS  
→

10/ 562,112



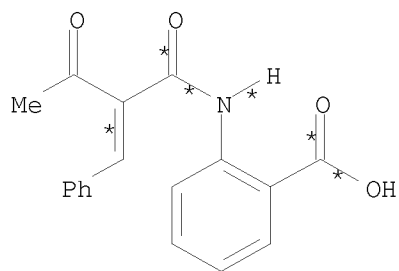
AV  
YIELD 70%

RX(1) RCT A 78817-80-8  
PRO B 70723-60-3  
CAT 108-24-7 Ac2O

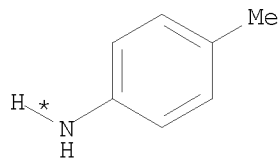
RX(10) RCT B 70723-60-3, P 62-53-3  
PRO Q 344572-47-0

RX(32) RCT Q 344572-47-0, AT 108-98-5  
PRO AV 78817-77-3

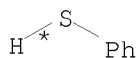
RX(84) OF 102 COMPOSED OF RX(1), RX(12), RX(33)  
RX(84) A + S + AT ==> AW



A



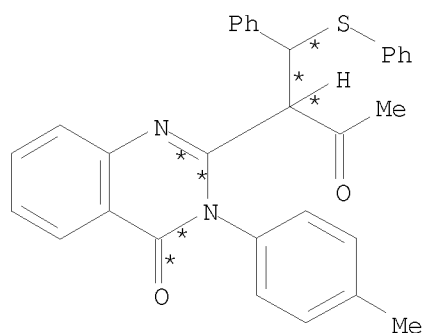
S



AT

3  
STEPS  
→

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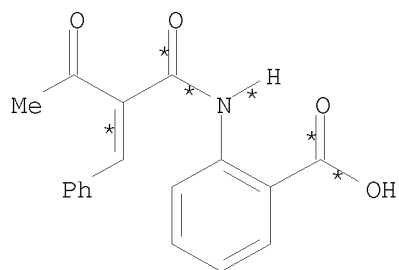
AW  
YIELD 70%

RX(1)      RCT    A 78817-80-8  
             PRO    B 70723-60-3  
             CAT    108-24-7 Ac2O

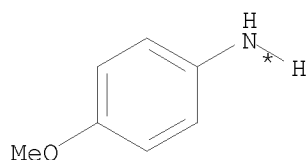
RX(12)     RCT    B 70723-60-3, S 106-49-0  
             PRO    T 344571-95-5

RX(33)     RCT    T 344571-95-5, AT 108-98-5  
             PRO    AW 78817-78-4

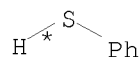
RX(87) OF 102 COMPOSED OF RX(1), RX(14), RX(34)  
RX(87)      A + V + AT ==> AX



A

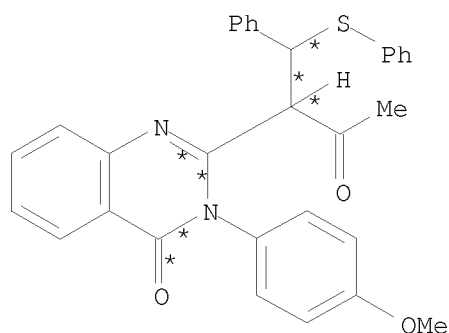


V



AT

3  
STEPS  
→



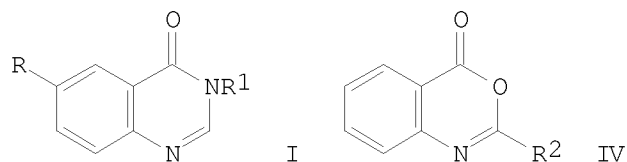
AX  
YIELD 70%

RX(1) RCT A 78817-80-8  
PRO B 70723-60-3  
CAT 108-24-7 Ac2O

RX(14) RCT B 70723-60-3, V 104-94-9  
PRO W 344580-68-3

RX(34) RCT W 344580-68-3, AT 108-98-5  
PRO AX 78817-79-5

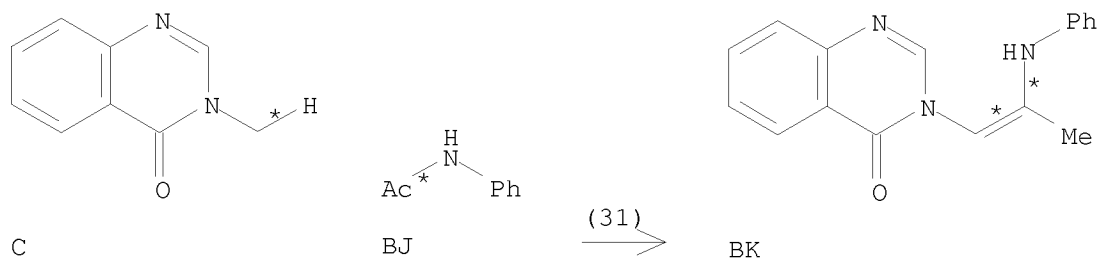
L3 ANSWER 217 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 95:115442 CASREACT  
TITLE: Reactions of some 4(3H)quinazolinones  
AUTHOR(S): Anwar, M.  
CORPORATE SOURCE: Fac. Sci., Tanta Univ., Tanta, Egypt  
SOURCE: Revue Roumaine de Chimie (1981), 26(4), 639-45  
CODEN: RRCHAX; ISSN: 0035-3930  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB The reaction of I (R = H, NO<sub>2</sub>; R<sub>1</sub> = H) with halo compds. gave I [R = H, R<sub>1</sub> = Me (II), Ac (III); R = NO<sub>2</sub>, R<sub>1</sub> = Me, Et, Ac, Bz, SO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Me-4]. III and IV (R<sub>2</sub> = Ph, CH:CHC<sub>6</sub>H<sub>4</sub>OMe-4, CH:CHC<sub>6</sub>H<sub>4</sub>Cl-2) underwent aminolysis. II underwent fusion with aldehydes, ketones, benzil, and anilides. II condensed with maleic, succinic, and phthalic anhydrides. III underwent condensation with aldehydes.

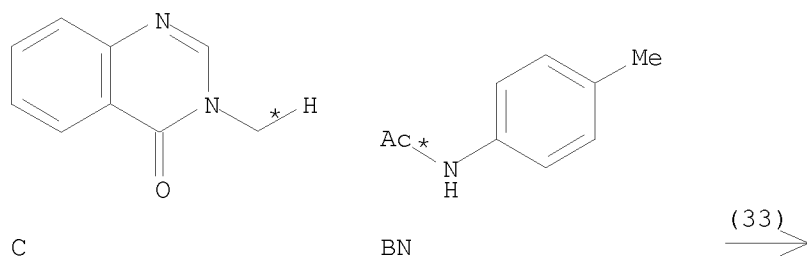


RX(31) OF 86 ...C + BJ ==&gt; BK



RX(31) RCT C 2436-66-0, BJ 103-84-4  
 PRO BK 78875-23-7

RX(33) OF 86 ...C + BN ==&gt; BO

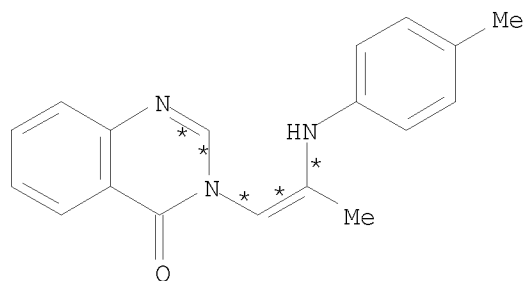


BO

RX(33) RCT C 2436-66-0, BN 103-89-9  
 PRO BO 78875-25-9

RX(62) OF 86 COMPOSED OF RX(1), RX(31)  
 RX(62) A + B + BJ ==> BK



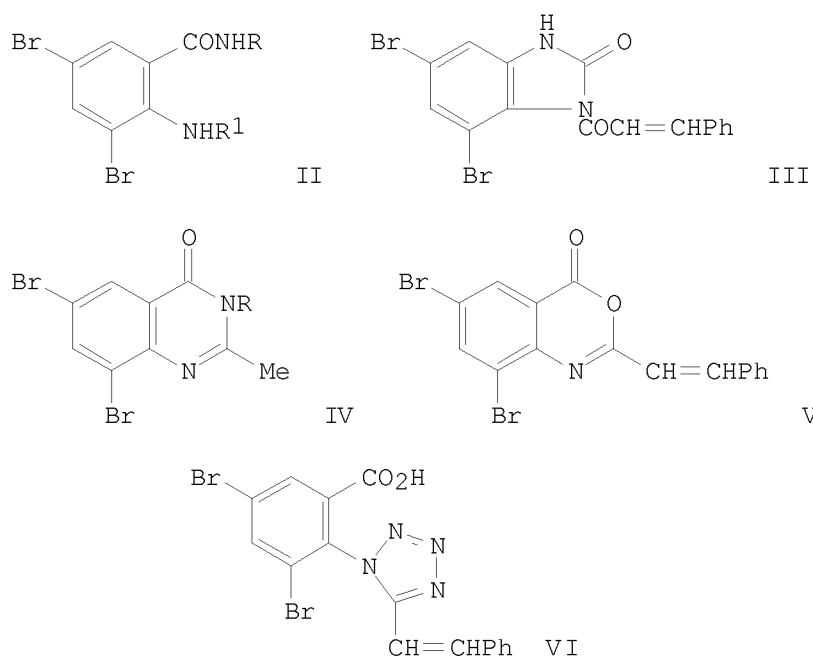


BO

RX(1) RCT A 491-36-1, B 74-88-4  
 PRO C 2436-66-0

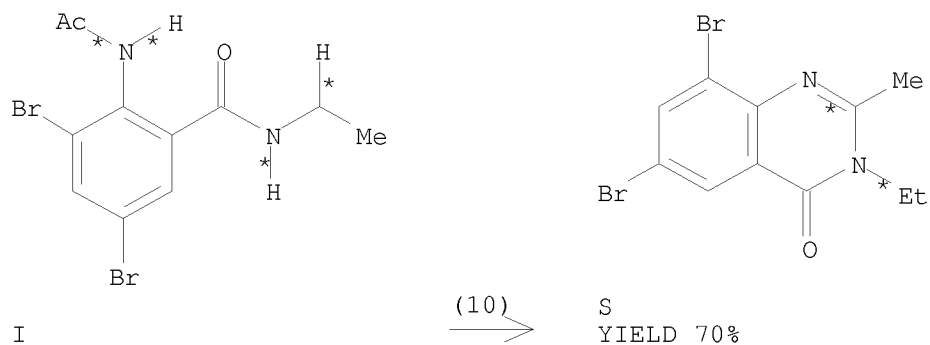
RX(33) RCT C 2436-66-0, BN 103-89-9  
 PRO BO 78875-25-9

L3 ANSWER 218 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 95:115418 CASREACT  
 TITLE: Reaction of 6,8-dibromo-2-methyl-3,1-benzoxazin-4(H)-one with some nucleophilic reagents: synthesis of quinazoline, tetrazole and benzimidazole derivatives  
 AUTHOR(S): Ismail, M. F.; Shams, N. A.; Naguib, M. I.  
 CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt  
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1981), 20B(5), 394-7  
 CODEN: IJSBDB; ISSN: 0376-4699  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB The reaction of 6,8-dibromo-2-methyl-3,1(4H)-benzoxazin-4-one (I) with RNH<sub>2</sub> (R = Et, Ph, NH<sub>2</sub>, NHPh, OH, NHCONH<sub>2</sub>) to give II (R<sub>1</sub> = Ac, PhCH:CH), and III. II (R<sub>1</sub> = Ac) cyclized to quinazolones IV. I condensed with PhCHO to give benzoxazine V, which was converted to II (R = CH<sub>2</sub>Ph, Ph; R<sub>1</sub> = COCH:CHPh). V treated with HN<sub>3</sub> gave VI and III.

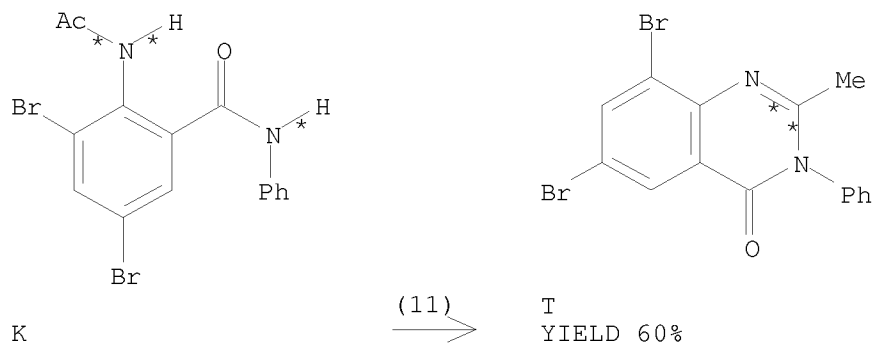
RX(10) OF 40 ...I ==> S...



RX(10) RCT I 78993-23-4  
PRO S 79008-15-4

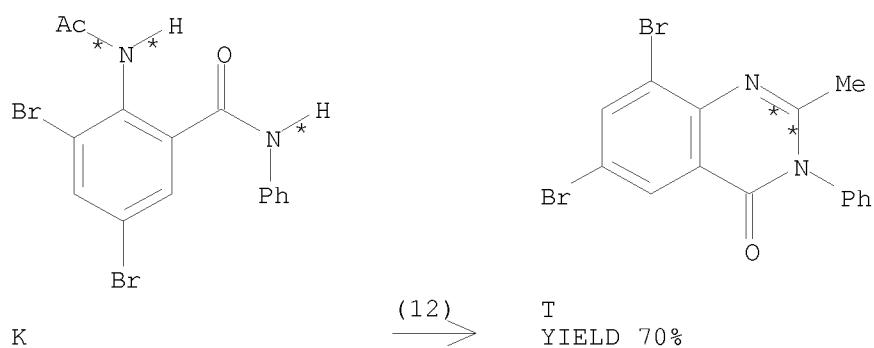
RX(11) OF 40 ...K ==> T...

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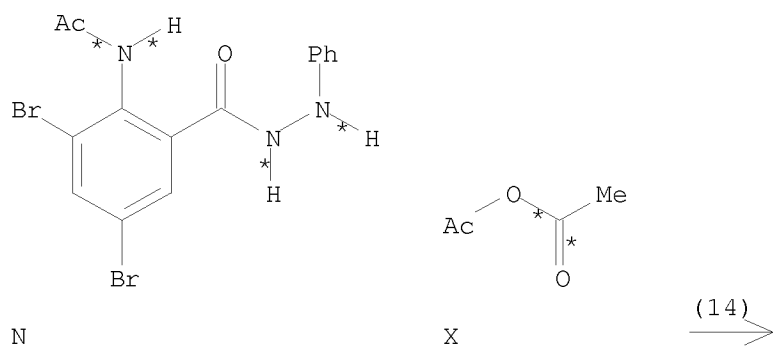
RX(11) RCT K 78993-24-5  
RGT U 10025-87-3 POC13  
PRO T 4145-21-5

RX(12) OF 40 K ==> T

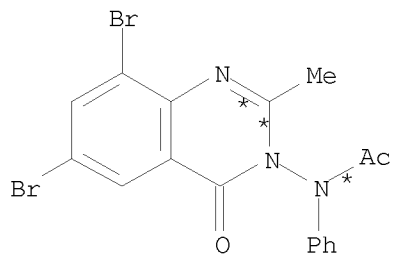


RX(12) RCT K 78993-24-5  
PRO T 4145-21-5

RX(14) OF 40 ...N + X ==> Y



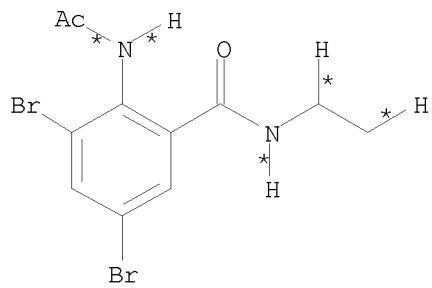
10/ 562,112



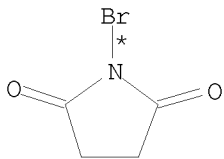
Y  
YIELD 72%

RX(14) RCT N 78993-26-7, X 108-24-7  
PRO Y 78993-29-0

RX(35) OF 40 COMPOSED OF RX(10), RX(15)  
 RX(35) I + Z ==> AA

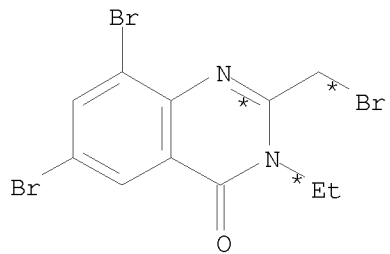


I



Z

2  
STEPS  
→



AA  
YIELD 22%

RX (10)	RCT	I	78993-23-4
	PRO	S	79008-15-4

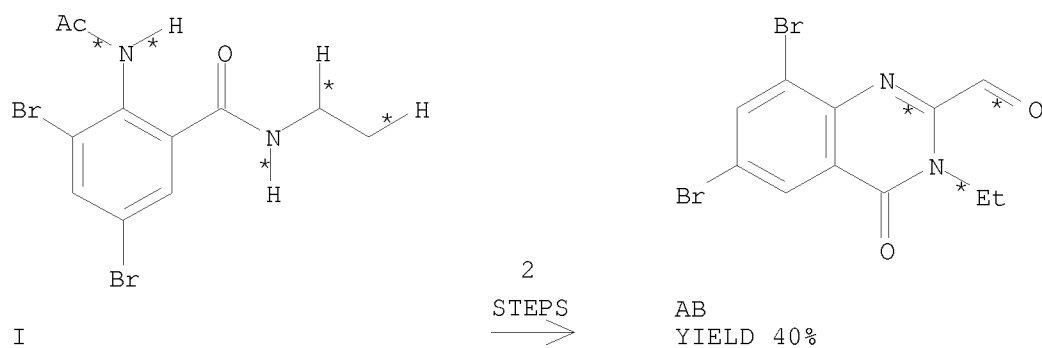
RX(15) RCT S 79008-15-4, Z 128-08-5

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PRO AA 78993-36-9

RX(36) OF 40 COMPOSED OF RX(10), RX(16)

RX(36) I ==> AB



RX(10) RCT I 78993-23-4

PRO S 79008-15-4

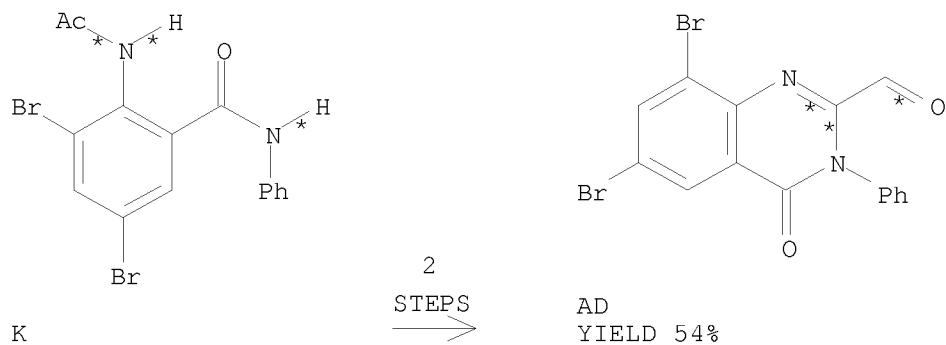
RX(16) RCT S 79008-15-4

RGT AC 7446-08-4 SeO2

PRO AB 78993-30-3

RX(37) OF 40 COMPOSED OF RX(11), RX(17)

RX(37) K ==> AD



RX(11) RCT K 78993-24-5

RGT U 10025-87-3 POC13

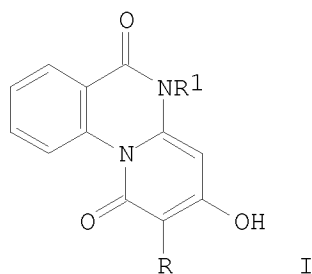
PRO T 4145-21-5

RX(17) RCT T 4145-21-5

RGT AC 7446-08-4 SeO2

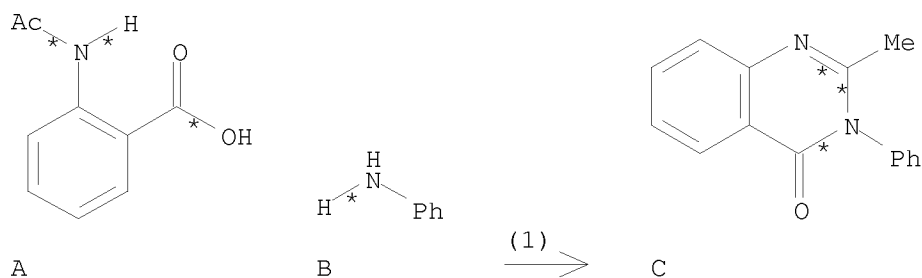
PRO AD 78993-31-4

L3 ANSWER 219 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 95:7205 CASREACT  
 TITLE: A new route to 1H-pyrido[1,2-a]quinazolines  
 AUTHOR(S): Soliman, Farid S. G.; Stadlbauer, Wolfgang; Kappe, Thomas  
 CORPORATE SOURCE: Fac. Pharm., Univ. Alexandria, Alexandria, Egypt  
 SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie (1981), 36B(2), 252-6  
 CODEN: ZNBAD2; ISSN: 0340-5087  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB The pyridoquinazolinones I ( $R = \text{PhCH}_2, \text{Et}, \text{Ph}, \text{Me}_2\text{CH}, \text{Bu}, R_1 = \text{Ph}, p\text{-BrC}_6\text{H}_4, o\text{-ClC}_6\text{H}_4, o\text{-MeC}_6\text{H}_4$ ) were prepared by reacting monosubstituted bis(2,4,6-trichlorophenyl) malonates with 3-aryl-3,4-dihydro-2-methyl-4-quinazolinones. Alkylation of I ( $R = R_1 = \text{Ph}$ ) with allyl bromide afforded the corresponding 3-allyloxy derivative. Certain generalizations of the cleavage processes of this series in the mass spectra are reported.

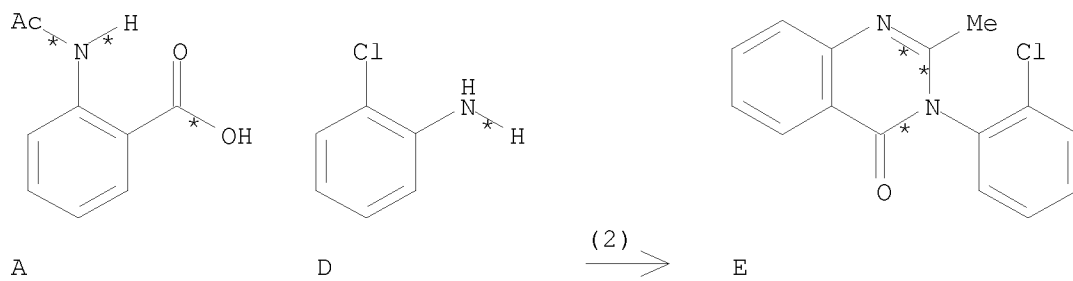
RX(1) OF 27 A + B ==> C...



RX(1) RCT A 89-52-1, B 62-53-3  
 PRO C 2385-23-1

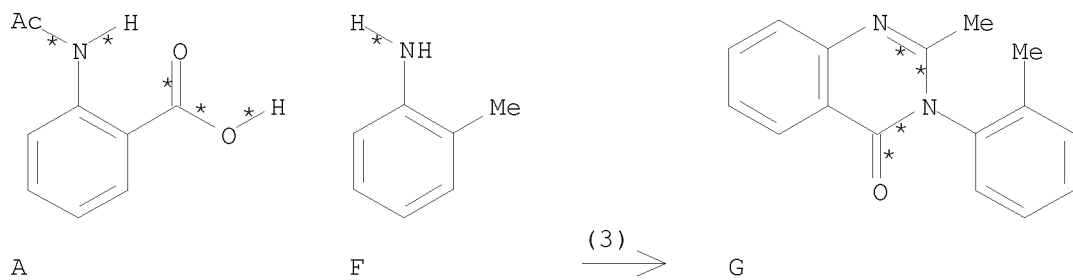
RX(2) OF 27 A + D ==> E...





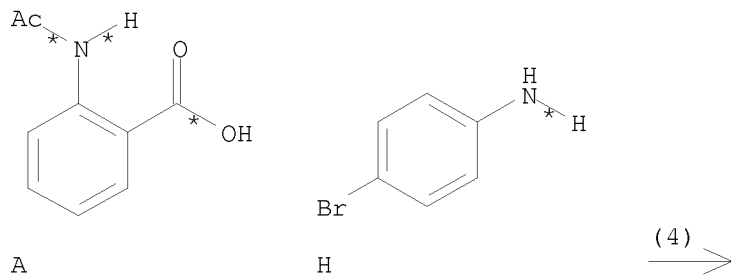
RX(2)      RCT    A 89-52-1, D 95-51-2  
              PRO    E 340-57-8

RX(3) OF 27      A + F  $\Rightarrow$  G...

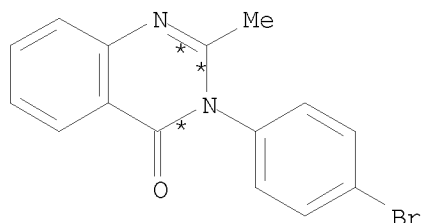


RX(3)      RCT    A 89-52-1, F 95-53-4  
              PRO    G 72-44-6

RX(4) OF 27      A + H  $\Rightarrow$  I...



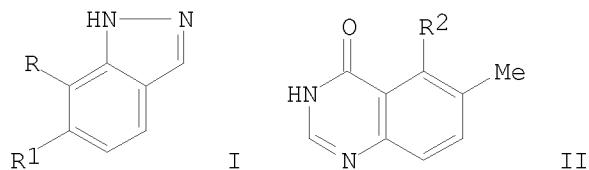
10/ 562,112



I  
YIELD 44%

RX(4) RCT A 89-52-1, H 106-40-1  
PRO I 1788-95-0

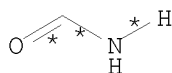
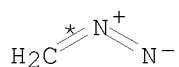
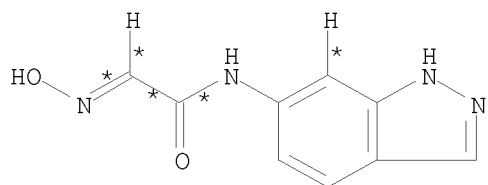
L3 ANSWER 220 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 95:7138 CASREACT  
TITLE: Nucleosides. Part 40. Synthesis of a [3,4-f]-linked  
pyrazoloquinazolinone  
AUTHOR(S): Lichtenthaler, Frieder W.; Cuny, Eckehard  
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Tech. Hochsch. Darmstadt,  
Darmstadt, D-6100, Fed. Rep. Ger.  
SOURCE: Heterocycles (1981), 15(2), 1053-9  
CODEN: HTCYAM; ISSN: 0385-5414  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB The pyrazoloquinazolinone I (RR1 = CONHCH:N) was prepared by 2 methods. Thus I (R = H, R1 = NH2) were treated with Cl3CCHO and NH2OH to give I (R = H, R1 = NHCOCH:NOH) which was cyclized with acid and oxidized with H2O2 to give I (R = CO2H, R1 = NH2). Esterification of acid and cyclization with HCONH2 gave I (RR1 = CONHCH:N). Alternatively II (R2 = H) was nitrated and II (R2 = NO2) reduced to the amine, diazotized, and cyclized with Me2NOAc.

RX(25) OF 26 COMPOSED OF RX(3), RX(4), RX(5), RX(2)  
RX(25) C + L + F ==> G

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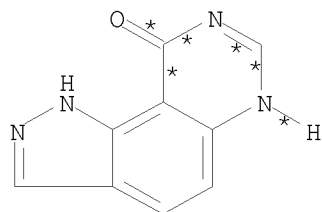


C

L

F

4  
STEPS  
→



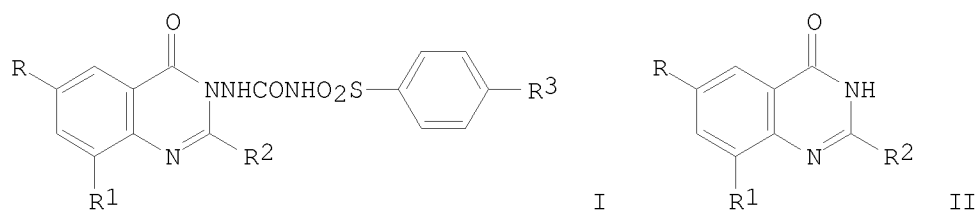
G

YIELD 74%

RX(3)	RCT	C	77929-34-1
	RGT	I	7664-93-9 H2SO4
	PRO	H	73907-94-5
RX(4)	RCT	H	73907-94-5
	RGT	K	7722-84-1 H2O2
	PRO	J	73907-95-6
RX(5)	RCT	J	73907-95-6, L 334-88-3
	PRO	E	73907-98-9
RX(2)	RCT	E	73907-98-9, F 75-12-7
	PRO	G	73907-90-1
	SOL		75-12-7 Formamide

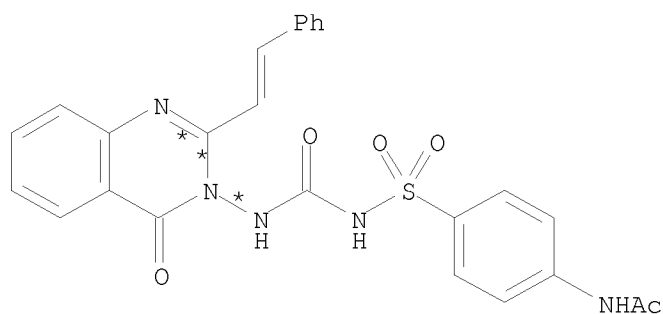
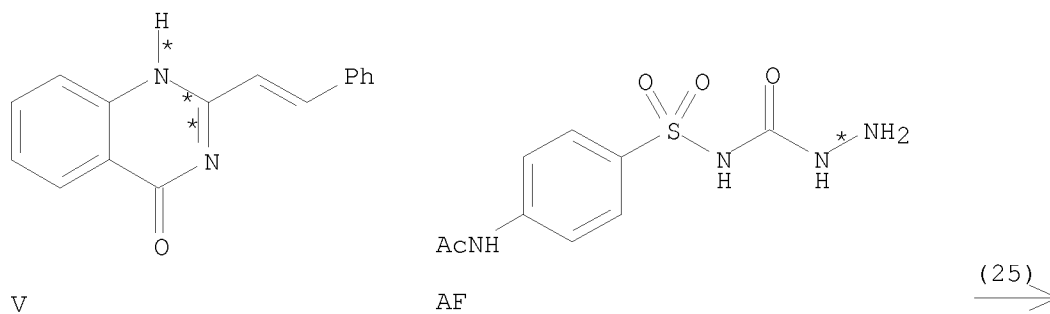
L3 ANSWER 221 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 94:139735 CASREACT  
TITLE: Synthesis of some new  
N1-(2-aryl-6,8-substituted-4-quinazolon-3-yl)-N8-

arylsulfonylureas as hypoglycemic agents  
 AUTHOR(S): Husain, M. Imtiaz; Srivastav, G. C.  
 CORPORATE SOURCE: Dep. Chem., Lucknow Univ., Lucknow, 226 007, India  
 SOURCE: Indian Journal of Chemistry, Section B: Organic  
 Chemistry Including Medicinal Chemistry (1980),  
 19B(10), 916-17  
 CODEN: IJSBDB; ISSN: 0376-4699  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Thirty two new compds. I (R, R1 = H, Br; R2 = Ph, 2,3,5-HOBr2C6H2, CH:CHPh; R3 = H, Me, MeO, NHAc) were prepared by refluxing II with 4-R3C6H4SO2NHCONH2 in pyridine. I (R = H, R1 = Br, R2 = Ph, R3 = NHAc) showed 38% reduction in blood sugar level in rats at an oral dose of 250 mg/kg.

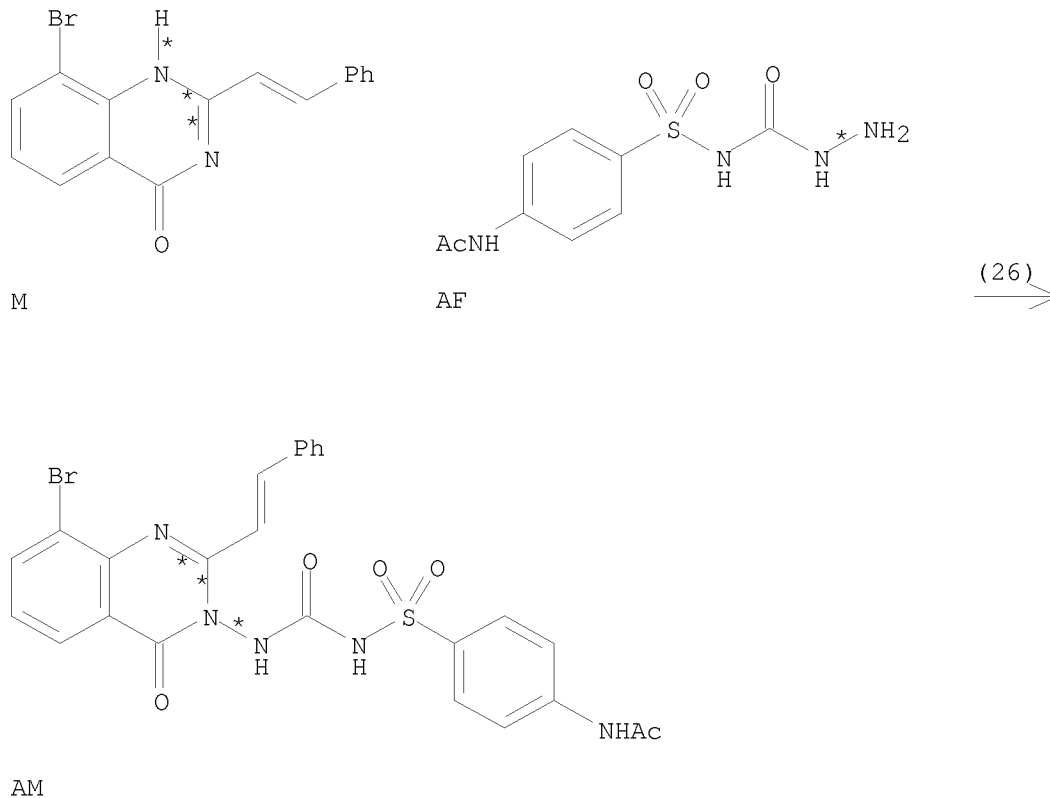
RX(25) OF 32 V + AF ==> AL



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RX(25) RCT V 4765-58-6, AF 76983-56-7  
PRO AL 344595-28-4  
CAT 110-86-1 Pyridine

RX(26) OF 32 M + AF ==> AM

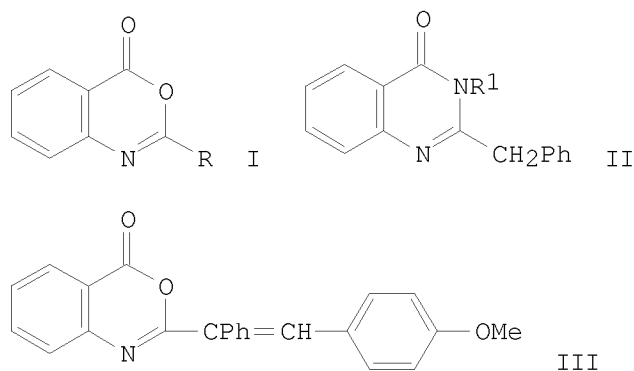


RX(26) RCT M 76983-54-5, AF 76983-56-7  
PRO AM 344608-04-4  
CAT 110-86-1 Pyridine

L3 ANSWER 222 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 94:139722 CASREACT  
TITLE: Some reactions with 2-benzyl-4H-3,1-benzoxazine-4-one,  
6-bromo-2-methyl-4H-3,1-benzoxazin-4-one and  
2-benzyl-3-phenyl-4 (3H)-quinazolinone  
AUTHOR(S): El Hashash, M. A.; Sayed, M. A.  
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt  
SOURCE: Egyptian Journal of Chemistry (1980), Volume Date  
1978, 21(2), 115-31  
CODEN: EGJCA3; ISSN: 0367-0422  
DOCUMENT TYPE: Journal

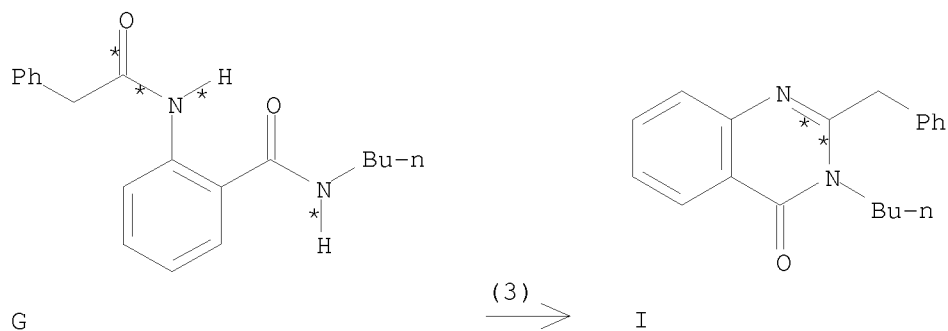
10/ 562,112

LANGUAGE: English  
GI



AB The benzoxazone I (R = PhCH<sub>2</sub>) reacted with primary amines R<sub>1</sub>NH<sub>2</sub> and gave o-R<sub>1</sub>NHCOC<sub>6</sub>H<sub>4</sub>NHCOCH<sub>2</sub>Ph (R<sub>1</sub> = Bu, PhCH<sub>2</sub>, p-HO<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>) and the quinazolinones II (R<sub>1</sub> = p-HOC<sub>6</sub>H<sub>4</sub>, Ph). Aldehydes and acetophenone condensed with I (R = PhCH<sub>2</sub>) and II (R<sub>1</sub> = Ph) and yielded styrylbenzoxazones, e.g. III and bisbenzoxazones. I (R = Ph) condensed with hydrazines, hydroxylamine and with active methylene compds. and yielded quinazolinones and a keto-ester, resp. Also, the reaction of I (R = Ph, Me) with aromatic hydrocarbons in presence of AlCl<sub>3</sub> and with aralkyl magnesium halides was described. P2S<sub>5</sub> reacted with I (R = Me) and yielded the corresponding thione.

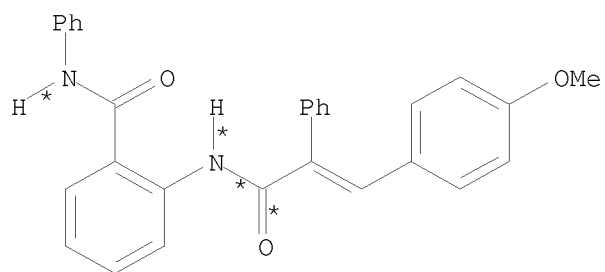
RX(3) OF 42 ...G ==> I



RX(3) RCT G 74772-51-3  
PRO I 74772-52-4  
CAT 108-24-7 Ac2O

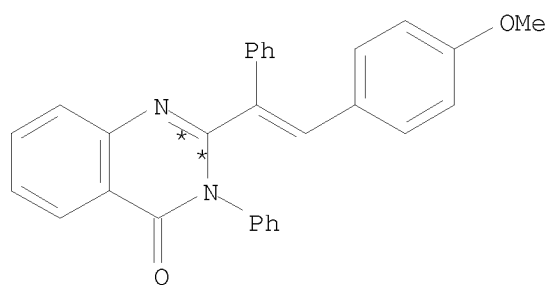
RX(10) OF 42 ...U ==> T

10/ 562,112



U

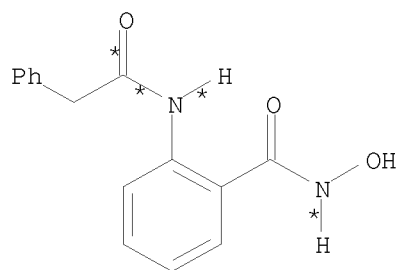
(10)  $\longrightarrow$



T

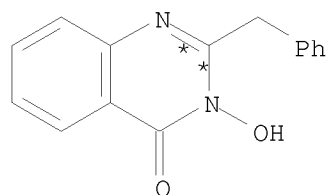
RX(10)      RCT    U 344610-95-3  
                  PRO    T 344610-14-6  
                  CAT    108-24-7 Ac2O

RX(14) OF 42      Z    ==>    AA



Z

(14)  $\longrightarrow$

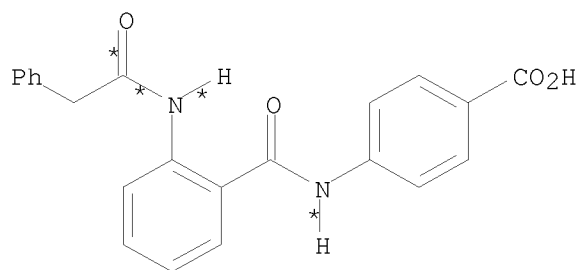


AA

RX(14)      RCT    Z 74772-63-7  
                  PRO    AA 74772-62-6  
                  CAT    108-24-7 Ac2O

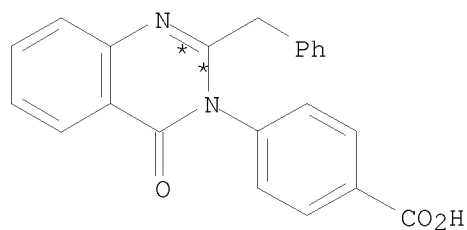
10/ 562,112

RX(17) OF 42      ...AF ==> AG



AF

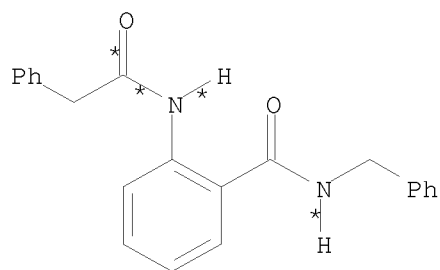
(17)



AG

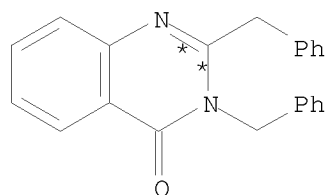
RX(17)      RCT    AF 76253-93-5  
             PRO    AG 76244-49-0  
             CAT    108-24-7 Ac2O

RX(20) OF 42      ...AI ==> AL



AI

(20)



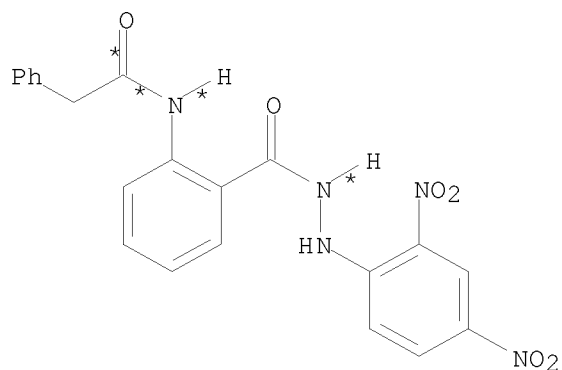
AL

RX(20)      RCT    AI 76253-92-4  
             PRO    AL 19857-42-2  
             CAT    108-24-7 Ac2O



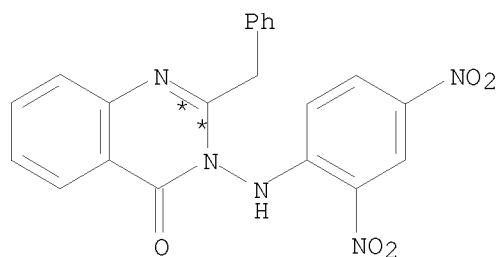
10/ 562,112

RX(24) OF 42 ...AR ==> AS



AR

(24) →

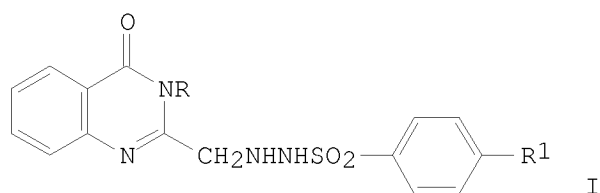


AS

RX(24)      RCT    AR 76254-00-7  
              PRO    AS 76253-99-1  
              CAT    108-24-7 Ac2O

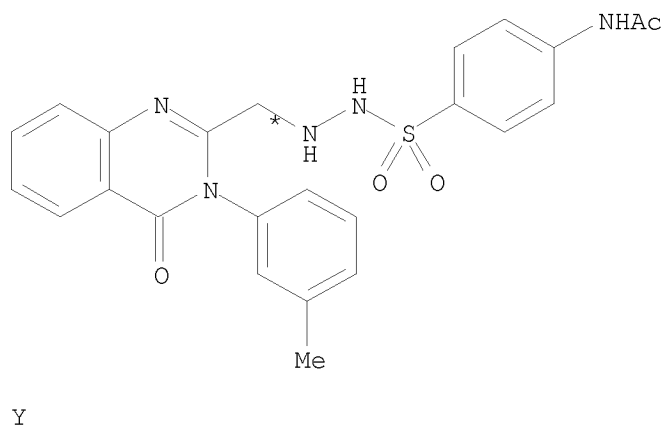
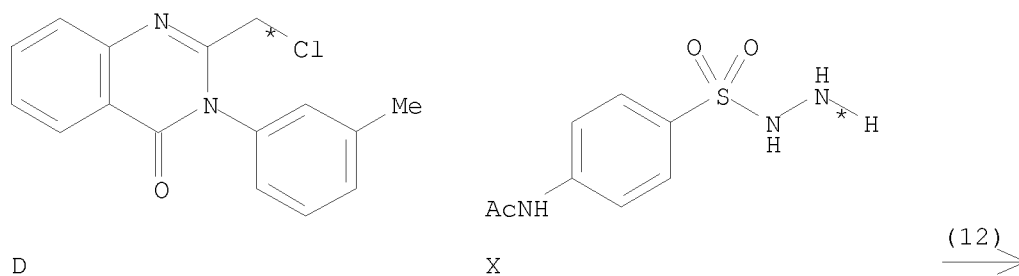
L3    ANSWER 223 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER:        94:84054    CASREACT  
TITLE:                    Quinazolinone derivatives of etiological interest.  
                             II.    Synthesis and antibacterial activity of certain  
                             3-aryl-2-(β-arylsulfonylhydrazinomethyl)-4(3H)-  
                             quinazolinones  
AUTHOR(S):                Abdel-Aleem, A. M.; Abdel-Ghaffar, A. F.  
CORPORATE SOURCE:        Fac. Pharm. Microbiol., Assiut Univ., Assiut, Egypt  
SOURCE:                    Indian Journal of Pharmaceutical Sciences (1980),  
                             42(3), 79-81  
                             CODEN: IJSIDW; ISSN: 0250-474X  
DOCUMENT TYPE:            Journal  
LANGUAGE:                  English  
GI

10/ 562,112



AB Quinazolinones I (R = 3-MeC6H4, 4-MeOC6H4, 4-ClC6H4, R1 = H, Me, NHAc, Br, Cl, NO2; R = Ph, 4-MeC6H4, 3-MeOC6H4, 4-BrC6H4, 3-ClC6H4, 4-EtO2CC6H4, 2-pyridyl, R1 = H) were prepared by treating the chloromethylquinazolinones with 4-R1C6H4SO2NHNH2. I had bactericidal activity less than that of sulfanilamide.

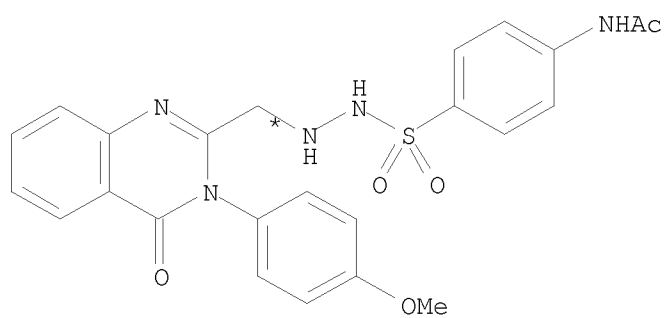
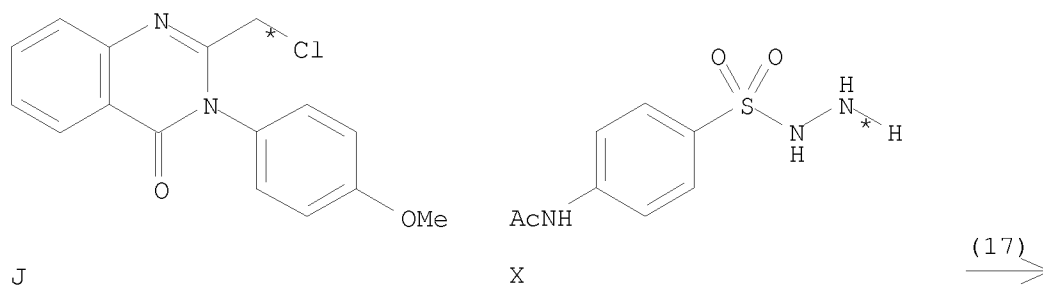
RX(12) OF 25 D + X ==> Y



RX(12) RCT D 22312-79-4, X 3989-50-2  
PRO Y 76534-89-9

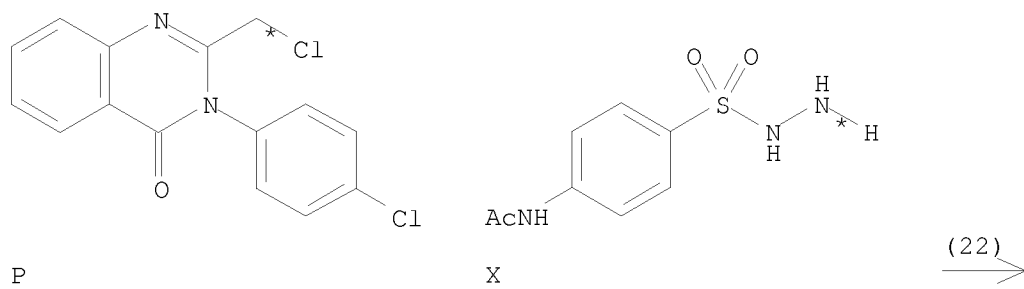
RX(17) OF 25 J + X ==> AG

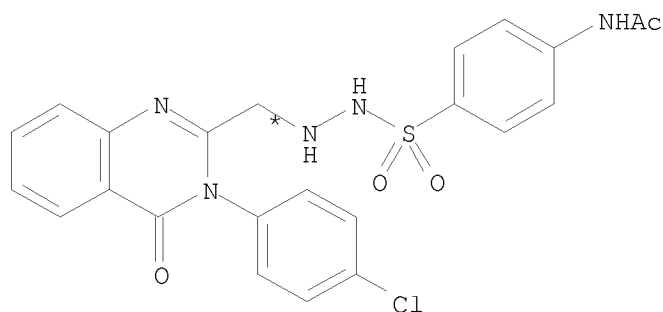
10/ 562,112



RX(17) RCT J 22312-82-9, X 3989-50-2  
PRO AG 76534-94-6

RX(22) OF 25 P + X ==> AL





AL

RX(22) RCT P 22280-87-1, X 3989-50-2  
 PRO AL 76534-99-1

L3 ANSWER 224 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 94:15765 CASREACT  
 TITLE: 4(3H)-Quinazolinones substituted with an aromatic  
 group in the 3 position  
 INVENTOR(S): Ishikawa, Masayuki; Tanaka, Hiromichi; Eguchi, Yukuo;  
 Ito, Shigeru; Takashima, Yoshimi; Kobayashi, Masahiko  
 PATENT ASSIGNEE(S): Japan  
 SOURCE: Ger. Offen., 58 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2950376	A1	19800710	DE 1979-2950376	19791214
JP 55083761	A	19800624	JP 1978-155764	19781219
JP 56051461	A	19810509	JP 1979-126738	19791003
JP 56057768	A	19810520	JP 1979-133582	19791018
JP 56065877	A	19810603	JP 1979-141987	19791105
US 4276295	A	19810630	US 1979-103841	19791214
SE 7910376	A	19800620	SE 1979-10376	19791217
AU 7953932	A	19800626	AU 1979-53932	19791217
AU 526309	B2	19830106		
DK 7905399	A	19800620	DK 1979-5399	19791218
NO 7904135	A	19800620	NO 1979-4135	19791218
NL 7909118	A	19800623	NL 1979-9118	19791218
GB 2040927	A	19800903	GB 1979-43565	19791218
GB 2040927	B	19830126		
BE 880720	A1	19800619	BE 1979-198633	19791219
FR 2444671	A1	19800718	FR 1979-31059	19791219
FR 2444671	B1	19830610		
ZA 7906892	A	19801231	ZA 1979-6892	19791219
DD 150462	A5	19810902	DD 1979-217854	19791219
CA 1111849	A1	19811103	CA 1979-342295	19791219

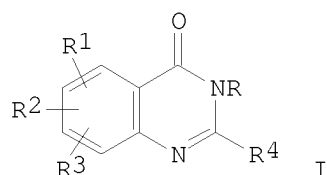
10/ 562,112

HU 25076	A2	19830530	HU 1979-II311	19791219
HU 182733	B	19840328		
AT 7908011	A	19840115	AT 1979-8011	19791219
AT 375651	B	19840827		
CH 644112	A5	19840713	CH 1979-11257	19791219

PRIORITY APPLN. INFO.:

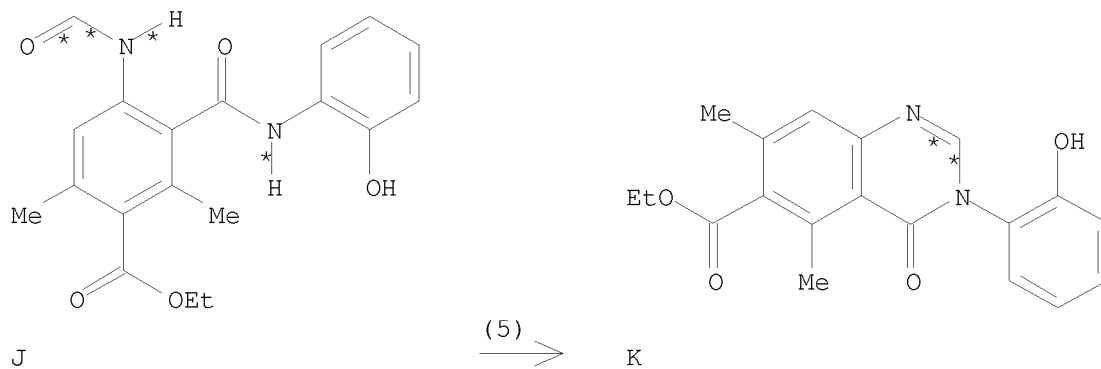
JP 1978-155764	19781219
JP 1979-126738	19791003
JP 1979-133582	19791018
JP 1979-141987	19791105

OTHER SOURCE(S): MARPAT 94:15765  
GI



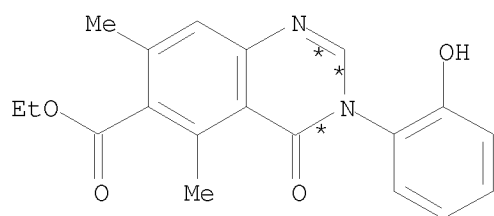
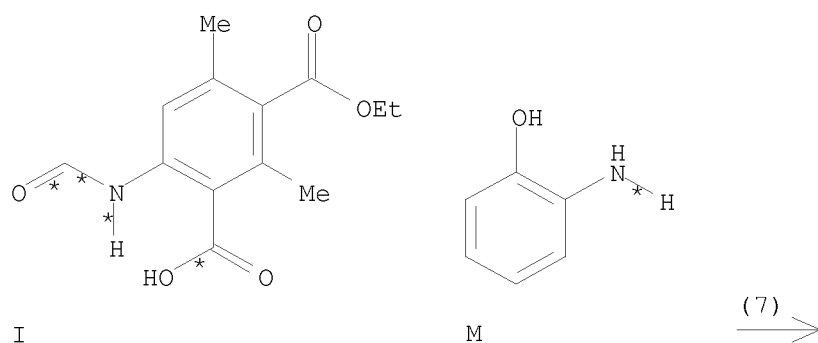
AB Quinazolinones I (R = optionally substituted Ph, pyridyl; R1, R3 = alkyl; R2 = alkoxy carbonyl; R4 = H, alkyl, halomethyl, CH2OAc, CH2OH) were prepared. Thus 2-amino-5-ethoxycarbonyl-4,6-dimethylbenzoic acid was treated with Ac2O to give 95% 6-ethoxycarbonyl-2,5,7-trimethyl-3,1,4-benzoxazone, which was treated with 2-MeC6H4NH2 to give 84.7% I (R = 2-MeC6H4, R1 = 5-Me, R2 = 6-CO2Et, R3 = 7-Me, R4 = Me, II). At  $3 \times 10^{-5}$  M II gave  $47 \pm 6.4\%$  relaxation of the thoracic artery in vitro.

RX(5) OF 10 J ==> K



RX(5) RCT J 345584-73-8  
PRO K 75913-00-7

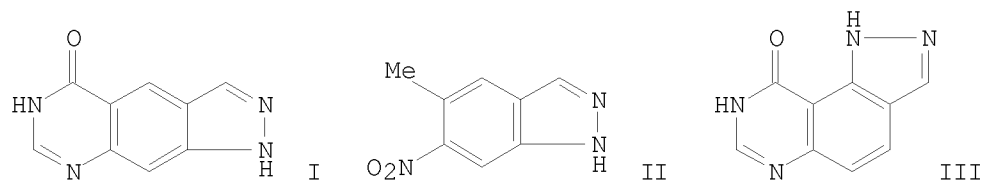
RX(7) OF 10 ...I + M ==> K



K

RX(7) RCT I 75913-88-1, M 95-55-6  
PRO K 75913-00-7

L3 ANSWER 225 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 94:3983 CASREACT  
TITLE: Nucleosides. 37. Benzologs of allopurinol: synthesis of pyrazolo[4,3-g] and [3,4-f]quinazolinones  
AUTHOR(S): Cuny, Eckehard; Lichtenthaler, F. W.; Moser, Alfred  
CORPORATE SOURCE: Inst. Org. Chem., Tech. Hochsch. Darmstadt, Darmstadt, D-6100, Fed. Rep. Ger.  
SOURCE: Tetrahedron Letters (1980), 21(32), 3029-32  
CODEN: TELEAY; ISSN: 0040-4039  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

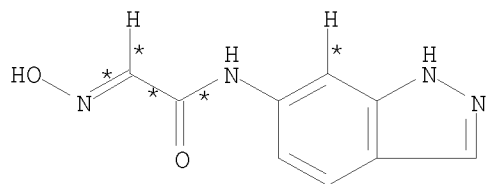


10/ 562,112

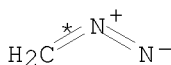
AB Pyrazoloquinazolinone I and its xanthine oxidase metabolite were prepared in 5 and 6 steps, resp., from indazole II, the key step being Niementowski type annulation of aminoindazolecarboxylic acids to give the pyrimidine ring. Two preps. of quinazolinone III by similar annulation, and by intramol. azo coupling (28% and 25% resp.) are reported.

RX(104) OF 120 COMPOSED OF RX(18), RX(19), RX(20), RX(4)

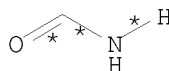
RX(104) X + L + B ==> G



X

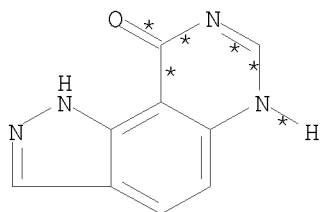


L



B

4  
STEPS  
→



G  
YIELD 74%

RX(18) RCT X 73907-93-4  
PRO Z 73907-94-5

RX(19) RCT Z 73907-94-5  
PRO AA 73907-95-6

RX(20) RCT AA 73907-95-6, L 334-88-3  
PRO F 73907-98-9

RX(4) RCT F 73907-98-9, B 75-12-7  
PRO G 73907-90-1

L3 ANSWER 226 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

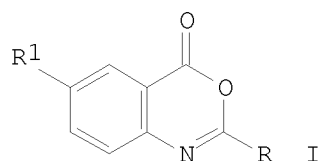
ACCESSION NUMBER: 93:114443 CASREACT

TITLE: Synthesis of new sulfamoyl anilides.  
4H-3,1-benzoxazin-4-one and 4-quinazolone derivatives  
of agricultural interest

AUTHOR(S): El-Hashash, M. A.; Mohamed, M. M.; Sayed, M. A.

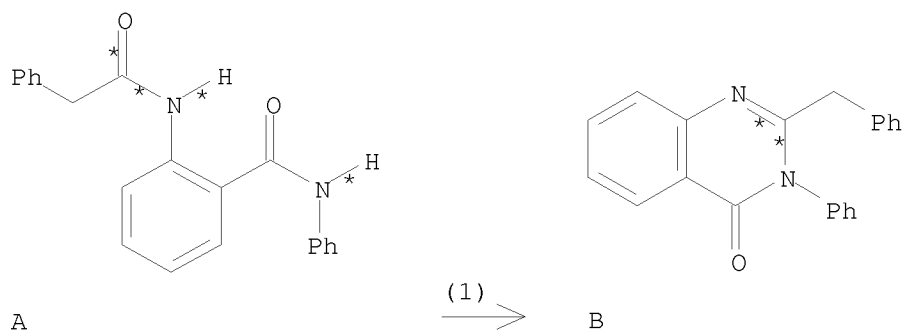
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt

SOURCE: Revue Roumaine de Chimie (1979), 24(11-12), 1509-20  
 CODEN: RRCHAX; ISSN: 0035-3930  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Benzoxazinones I ( $R = \text{CH}_2\text{Ph}$ ,  $R_1 = \text{H}$ ;  $R = \text{Me}$ ,  $R_1 = \text{Br}$ ) reacted with sulfa compds., amines, aldehydes, hydrazines,  $\text{NH}_2\text{OH}$ , and active methylene compds. to give side chain-substituted benzoxazinones, quinazolones, and acylaminobenzoyl derivs. The products had herbicidal activity, but were generally ineffective as insecticides, fungicides, bactericides, and virucides.

RX(1) OF 44 ...A ==> B...

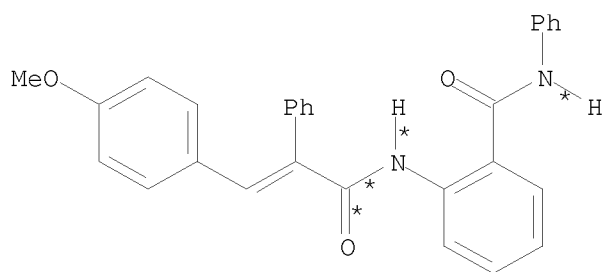


RX(1) RCT A 74772-50-2  
 PRO B 19857-34-2  
 CAT 108-24-7 Ac20

RX(20) OF 44 ...AL ==> AM

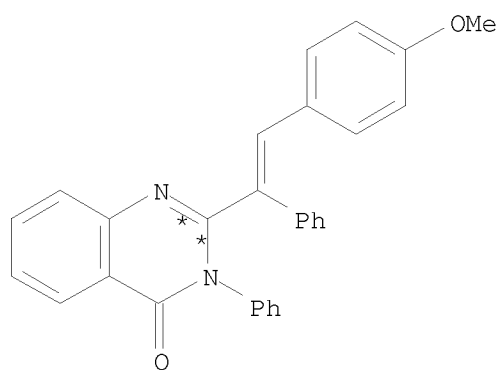


10/ 562,112



AL

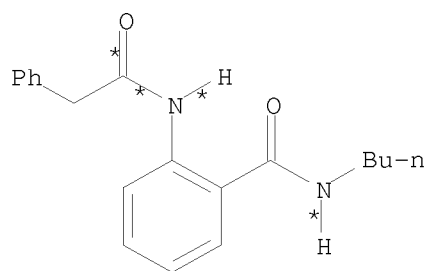
(20)



AM

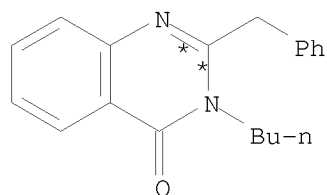
RX(20)      RCT    AL 74772-65-9  
                  PRO    AM 74772-58-0  
                  CAT    108-24-7 Ac2O

RX(31) OF 44      ...AA ==> BB



AA

(31)



BB

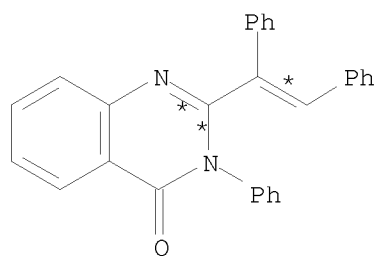
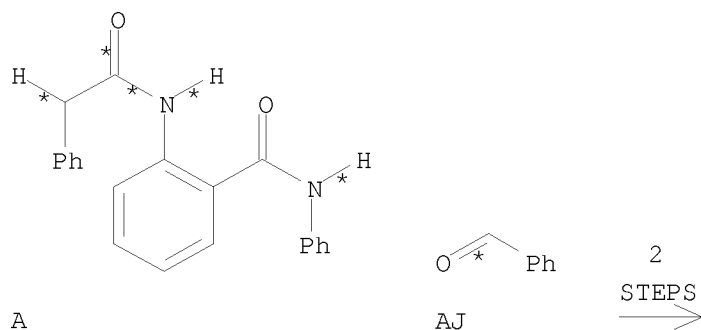
RX(31)      RCT    AA 74772-51-3  
                  PRO    BB 74772-52-4

10/ 562,112

CAT 108-24-7 Ac2O

RX(35) OF 44 COMPOSED OF RX(1), RX(19)

RX(35) A + AJ ==> AK



AK

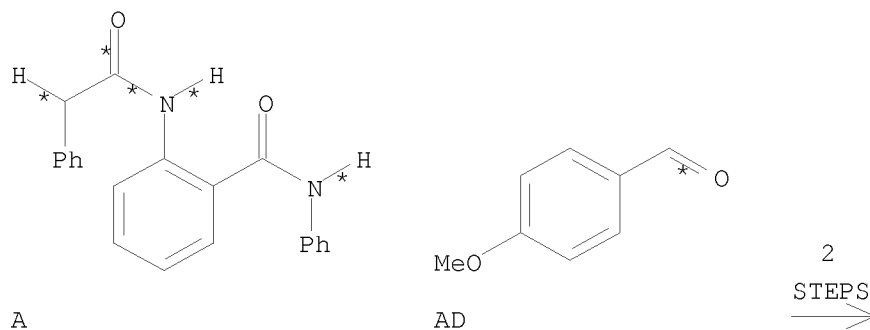
YIELD 65%

RX(1) RCT A 74772-50-2  
PRO B 19857-34-2  
CAT 108-24-7 Ac2O

RX(19) RCT B 19857-34-2, AJ 100-52-7  
PRO AK 74772-57-9

RX(36) OF 44 COMPOSED OF RX(1), RX(32)

RX(36) A + AD ==> AM

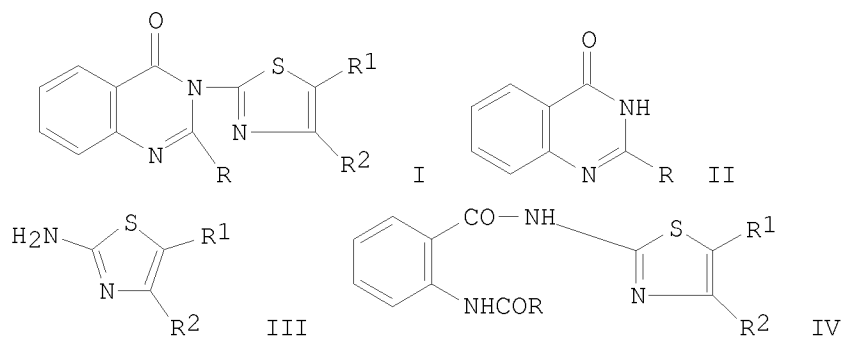


AM  
YIELD 58%

RX(1) RCT A 74772-50-2  
PRO B 19857-34-2  
CAT 108-24-7 Ac2O

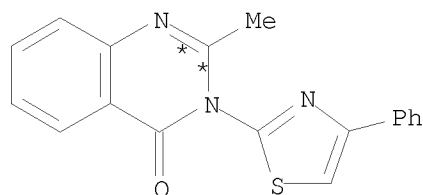
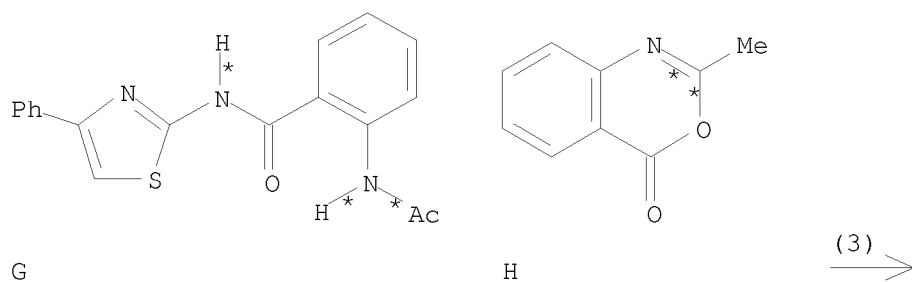
RX(32) RCT B 19857-34-2, AD 123-11-5  
PRO AM 74772-58-0

L3 ANSWER 227 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 93:95222 CASREACT  
TITLE: Synthesis of thiazolylquinazolin-4(3H)-ones  
AUTHOR(S): Badr, M. Z. A.; El-Sherief, H. A. H.; El-Naggar, G. M.; Mahmoud, A. M.  
CORPORATE SOURCE: Fac. Sci., Assiut Univ., Assiut, Egypt  
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1979), 18B(6), 560-3  
CODEN: IJSBDB; ISSN: 0376-4699  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB 3-Thiazolylquinazolin-4-ones I (R = Me, Ph; R<sub>1</sub> = H, CO<sub>2</sub>Et; R<sub>2</sub> = Ph, 4-MeC<sub>6</sub>H<sub>4</sub>, 4-MeOC<sub>6</sub>H<sub>4</sub>, 4-ClC<sub>6</sub>H<sub>4</sub>, 4-BrC<sub>6</sub>H<sub>4</sub>, Me) were prepared by condensing 3,1-benzoxazin-4(H)-ones II with aminothiazoles III. Heating 2-arylaminothiazoles IV in dry pyridine also give I. 2-Styrylquinazolin-4-ones I (R = 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CH:CH, R<sub>1</sub> = H, Ph, CO<sub>2</sub>Et, R<sub>2</sub> = Ph, Me, 4-MeC<sub>6</sub>H<sub>4</sub>; R = 4-ClC<sub>6</sub>H<sub>4</sub>CH:CH, R<sub>1</sub> = R<sub>2</sub> = Ph) were prepared by condensing aromatic aldehydes with I (R = Me). I and IV showed bactericidal activity.

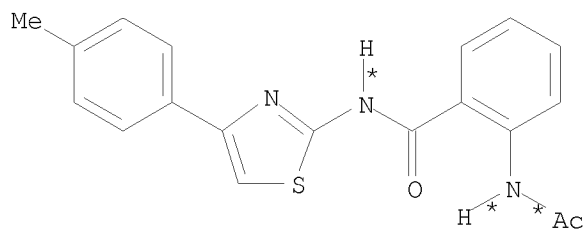
RX(3) OF 33            G + H ==> I...



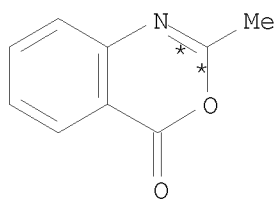
RX(3)            RCT    G 74636-72-9, H 525-76-8  
                   PRO    I 74636-80-9

RX(5) OF 33            J + H ==> K...

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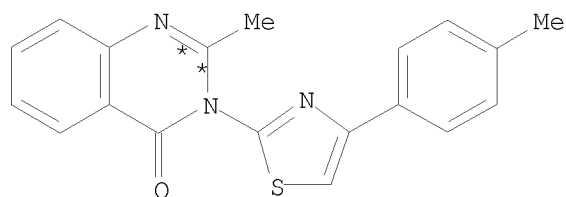


J



H

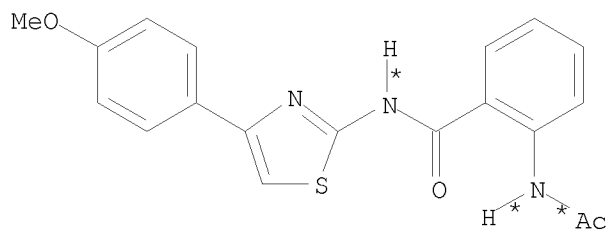
(5)  $\longrightarrow$



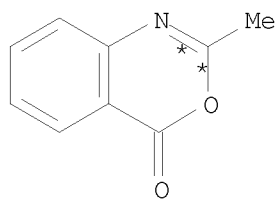
K

RX (5) RCT J 74636-73-0, H 525-76-8  
PRO K 74636-85-4

RX (7) OF 33 M + H  $\implies$  N

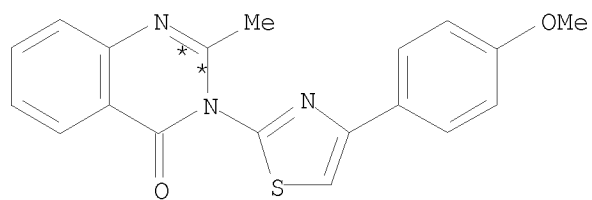


M



H

(7)  $\longrightarrow$

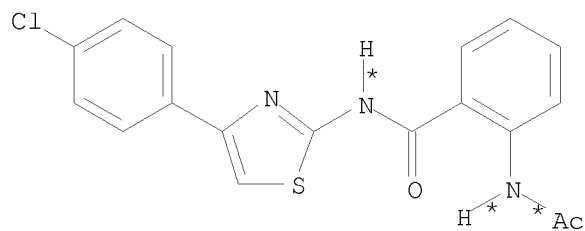


N

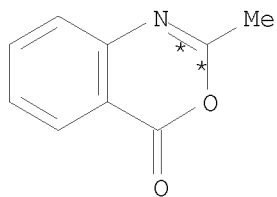
RX (7) RCT M 74636-74-1, H 525-76-8  
PRO N 74636-81-0

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RX(9) OF 33      P + H ==> Q

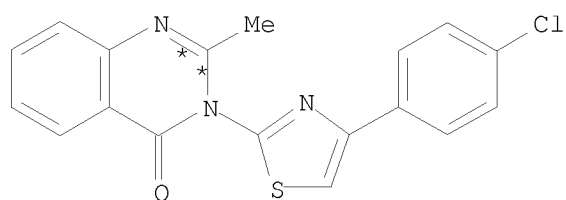


P



H

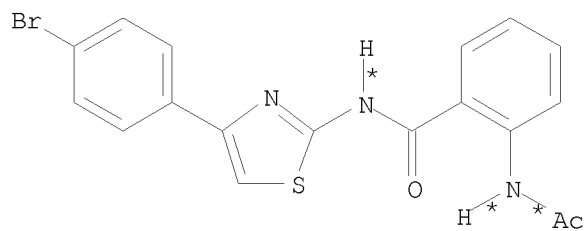
(9)  $\longrightarrow$



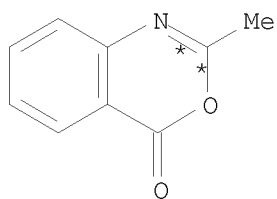
Q

RX(9)      RCT    P 74636-75-2, H 525-76-8  
PRO    Q 74636-82-1

RX(11) OF 33      S + H ==> T

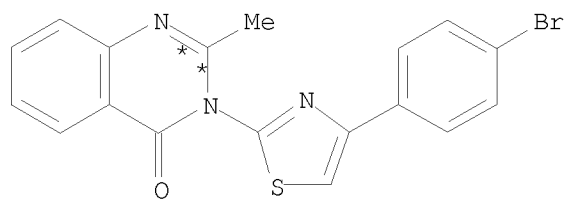


S



H

(11)  $\longrightarrow$

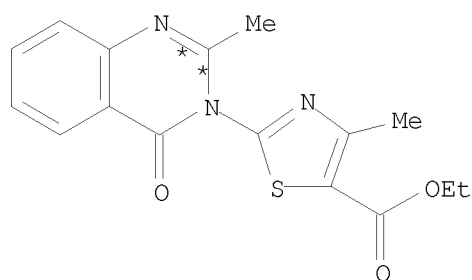
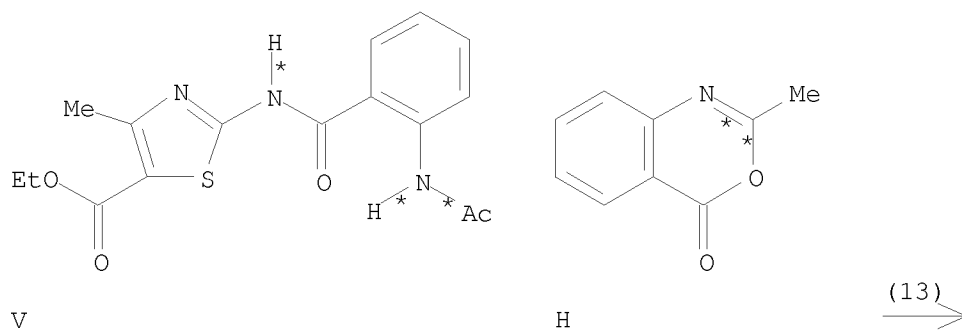


T

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RX(11) RCT S 74636-76-3, H 525-76-8  
PRO T 74636-83-2

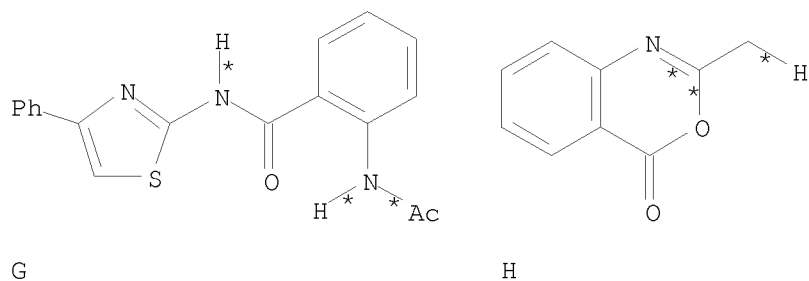
RX(13) OF 33 V + H ==> W...



W

RX(13) RCT V 74636-77-4, H 525-76-8  
PRO W 74636-84-3

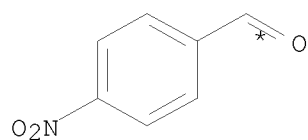
RX(26) OF 33 COMPOSED OF RX(3), RX(22)  
RX(26) G + H + AF ==> AH



G

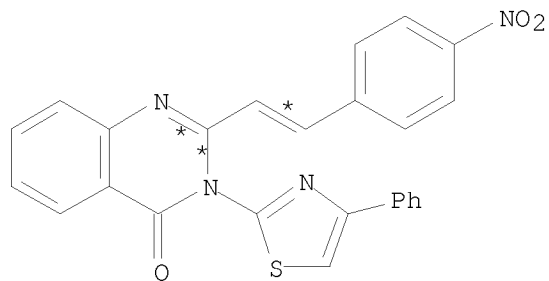
H

10/ 562,112



AF

2  
STEPS  
→

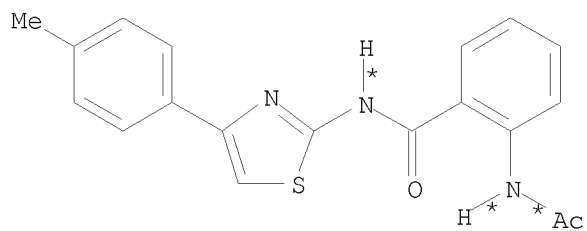


AH

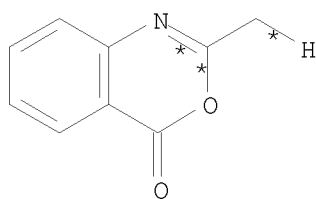
RX(3) RCT G 74636-72-9, H 525-76-8  
PRO I 74636-80-9

RX(22) RCT I 74636-80-9, AF 555-16-8  
PRO AH 74636-93-4

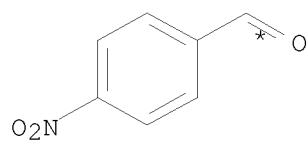
RX(28) OF 33 COMPOSED OF RX(5), RX(23)  
RX(28) J + H + AF ==> AI



J



H

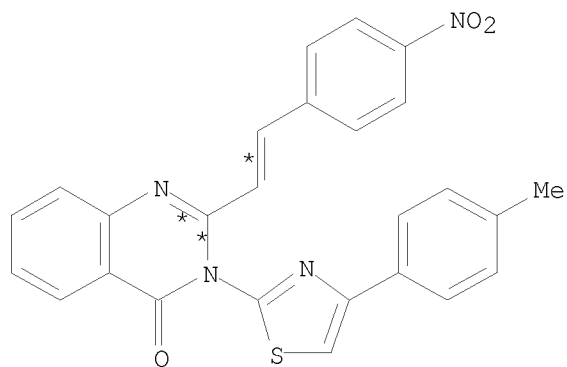


AF

2  
STEPS  
→



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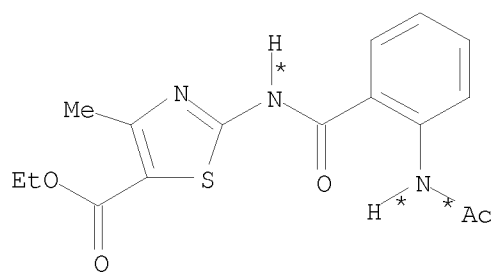


AI

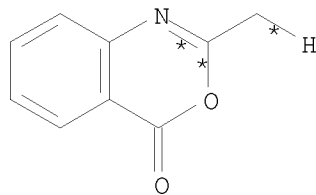
RX(5) RCT J 74636-73-0, H 525-76-8  
PRO K 74636-85-4

RX(23) RCT K 74636-85-4, AF 555-16-8  
PRO AI 74636-96-7

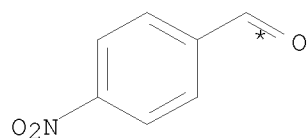
RX(30) OF 33 COMPOSED OF RX(13), RX(24)  
RX(30) V + H + AF ==> AJ



V

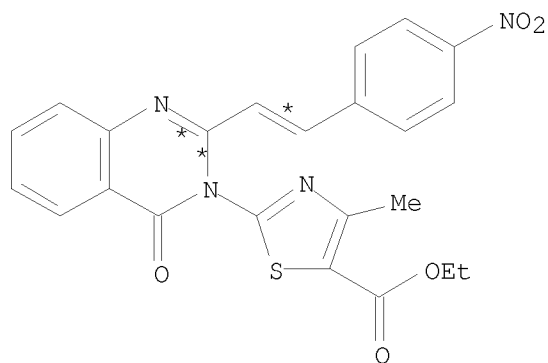


H



AF

2  
STEPS  
→

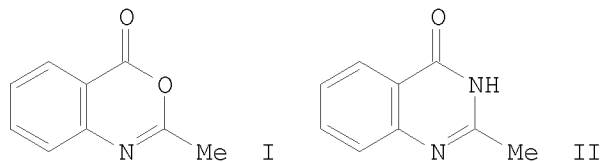


AJ

RX(13) RCT V 74636-77-4, H 525-76-8  
PRO W 74636-84-3

RX(24) RCT W 74636-84-3, AF 555-16-8  
PRO AJ 74636-94-5

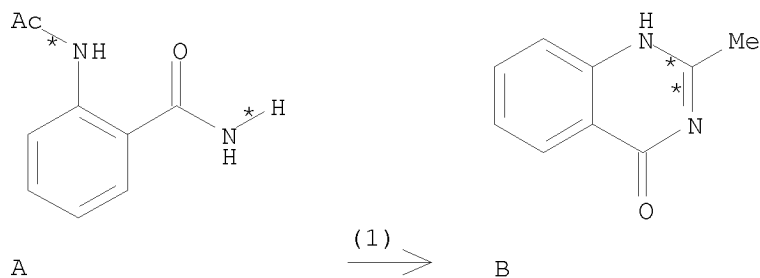
L3 ANSWER 228 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 93:70766 CASREACT  
TITLE: Acylantranils. 9. Influence of hydrogen bonding on the reaction of acetylanthranil with ammonia  
AUTHOR(S): Errede, L. A.; Martinucci, P. D.; McBrady, J. J.  
CORPORATE SOURCE: Res. Lab., 3M, St. Paul, MN, 55133, USA  
SOURCE: Journal of Organic Chemistry (1980), 45(15), 3009-17  
CODEN: JOCEAH; ISSN: 0022-3263  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB H bonding has a marked influence on the reaction of acetylanthranil (I) with NH<sub>3</sub>. The product of the reaction in anhydrous C<sub>6</sub>H<sub>6</sub> is the quinazolinone II, but the rate of formation is unusually slow. The rate of this conversion is about 6 times faster in pyridine than in C<sub>6</sub>H<sub>6</sub>. If H<sub>2</sub>O is added to the C<sub>6</sub>H<sub>6</sub> system, the rate of reaction is increased by orders of magnitude, but the product is o-AcNHC<sub>6</sub>H<sub>4</sub>CONH<sub>2</sub> (III). In contrast, addition of H<sub>2</sub>O to the pyridine system causes a small decrease in the rate and only a slight change in selectivity. These results are consistent with postulated mechanisms whereby I reacts with mol. clusters of NH<sub>3</sub>, i.e.,

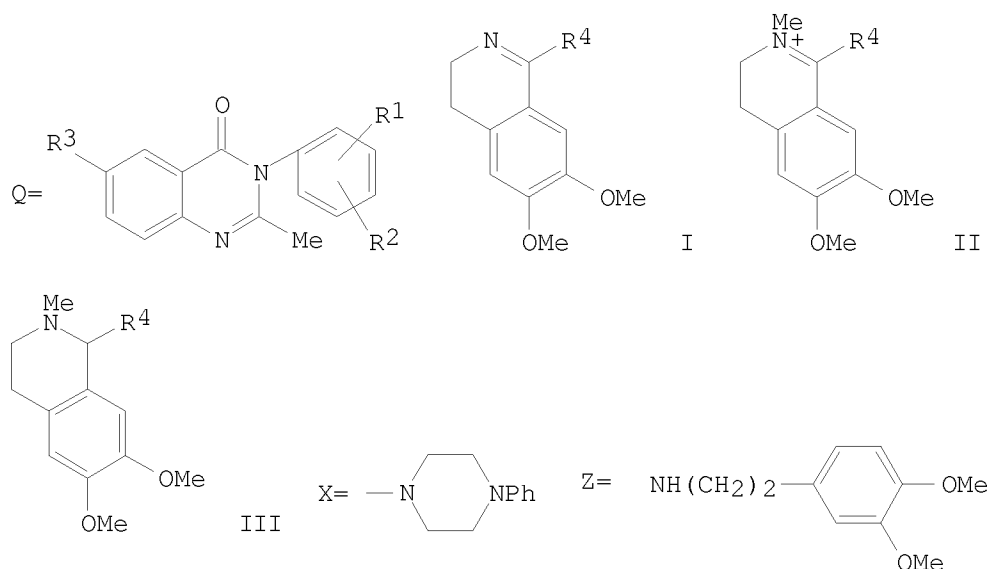
with (NH<sub>3</sub>)<sub>n</sub> in C<sub>6</sub>H<sub>6</sub>, with N(H·S)<sub>3</sub> in strong proton-acceptor solvents S, and with (NH<sub>3</sub>)<sub>n</sub>.H<sub>2</sub>O in C<sub>6</sub>H<sub>6</sub> containing added H<sub>2</sub>O. III underwent cyclodehydration to give II.

RX(1) OF 4 ...A ==> B



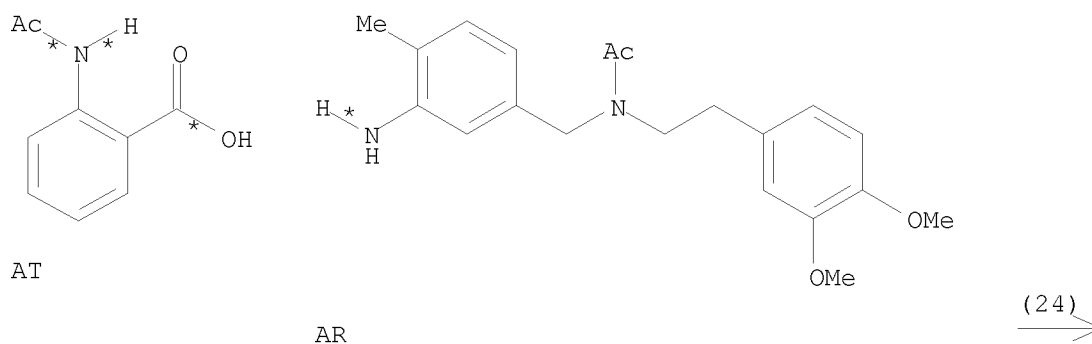
RX(1)        RCT    A 33809-77-7  
               PRO    B 1769-24-0

L3    ANSWER 229 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER:        93:46560    CASREACT  
 TITLE:                    Drugs acting on CNS: syntheses of  
                               2-methyl-3-o-tolylquinazolin-4-one (methaqualone)  
                               analogs  
 AUTHOR(S):                Prasad, Rajendra; Bhaduri, A. P.  
 CORPORATE SOURCE:        Div. Med. Chem., Cent. Drug Res. Inst., Lucknow,  
                               226001, India  
 SOURCE:                    Indian Journal of Chemistry, Section B: Organic  
                               Chemistry Including Medicinal Chemistry (1979),  
                               18B(5), 443-8  
                               CODEN: IJSBDB; ISSN: 0376-4699  
 DOCUMENT TYPE:            Journal  
 LANGUAGE:                 English  
 GI

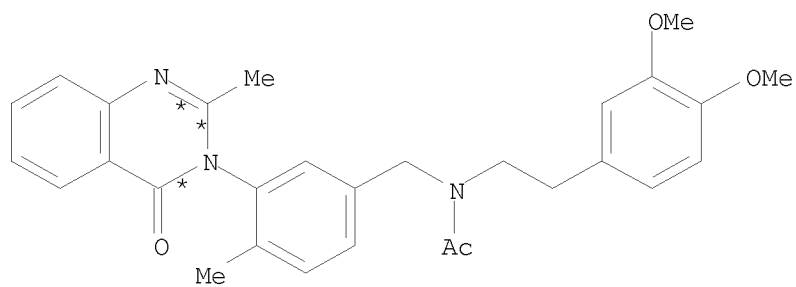


AB 3-Aryl-2-methyl-4(3H)-quinazolones [QH, QCO<sub>2</sub>H, QC1 (R<sup>1</sup> = H, R<sup>2</sup> = 2-Cl, 3-Cl, 2-Me, 4-F; 4-Br; R<sup>1</sup> = R<sup>2</sup> = 3-Me; R<sup>3</sup> = iodo, H)] were prepared in 53-93% yields. Cyclization of QCONH(CH<sub>2</sub>)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>(OMe)<sub>2-3,4</sub> followed sequentially by iodomethylation of I [R<sup>4</sup> = Q (R<sup>1</sup> = 2-Me, R<sup>2</sup> = R<sup>3</sup> = H)] and NaBH<sub>4</sub> reduction of II [R<sup>4</sup> = Q (R<sup>1</sup> = 2-Me, R<sup>2</sup> = R<sup>3</sup> = H)] gave III [R<sup>4</sup> = Q (R<sup>1</sup> = 2-Me, R<sup>2</sup> = R<sup>3</sup> = H)]. Condensation of 2,5-Me(XCH<sub>2</sub>)C<sub>6</sub>H<sub>3</sub>NH<sub>2</sub> and 2-AcNHC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H in the presence of dicyclohexylcarbodiimide gave QH (R<sup>1</sup> = 2-Me, R<sup>2</sup> = 5-XCH<sub>2</sub>, R<sup>3</sup> = H). Also prepared was QH (R<sup>1</sup> = 2-Me, R<sup>2</sup> = CH<sub>2</sub>Z, R<sup>3</sup> = H). None of the compds. possessed any central nervous system depressant activity. The LD<sub>50</sub> of the compds. was >1000 mg/kg i.p.

RX(24) OF 58 ...AT + AR ==> AU...



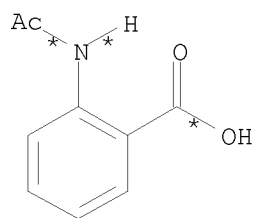
10/ 562,112



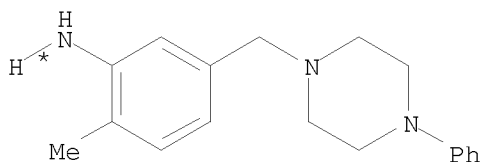
AU

RX(24)      RCT    AT 89-52-1, AR 74101-73-8  
              PRO    AU 74101-74-9  
              CAT    538-75-0 DCC

RX(25) OF 58      ...AT + AQ ==> AW

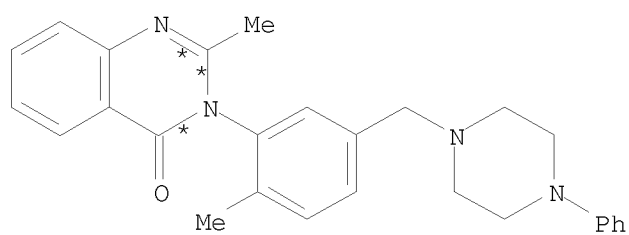


AT



AQ

(25) ➞

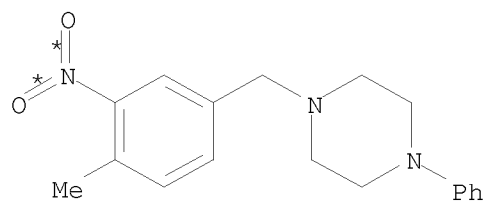


AW

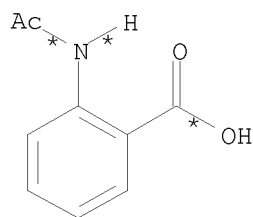
RX(25)      RCT    AT 89-52-1, AQ 74101-72-7  
              PRO    AW 74101-75-0  
              CAT    538-75-0 DCC

RX(41) OF 58 COMPOSED OF RX(22), RX(25)  
RX(41)      AM + AT ==> AW

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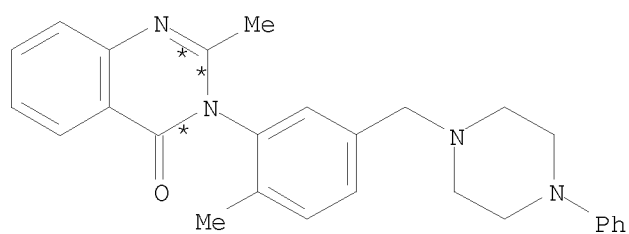


AM



AT

2  
STEPS  
→

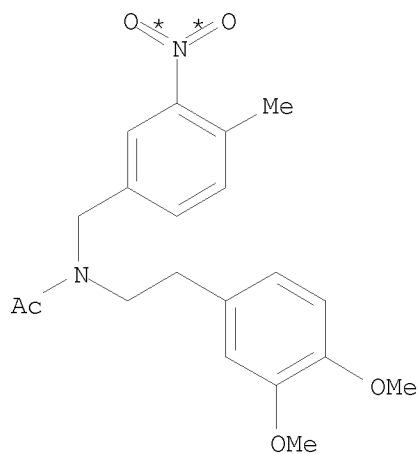


AW

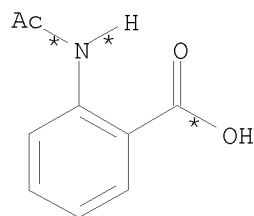
RX(22) RCT AM 74101-69-2  
PRO AQ 74101-72-7

RX(25) RCT AT 89-52-1, AQ 74101-72-7  
PRO AW 74101-75-0  
CAT 538-75-0 DCC

RX(42) OF 58 COMPOSED OF RX(23), RX(24)  
RX(42) AP + AT ==> AU



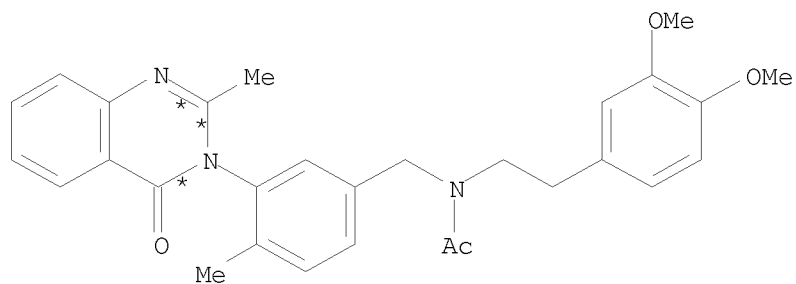
AP



AT

2  
STEPS  
→

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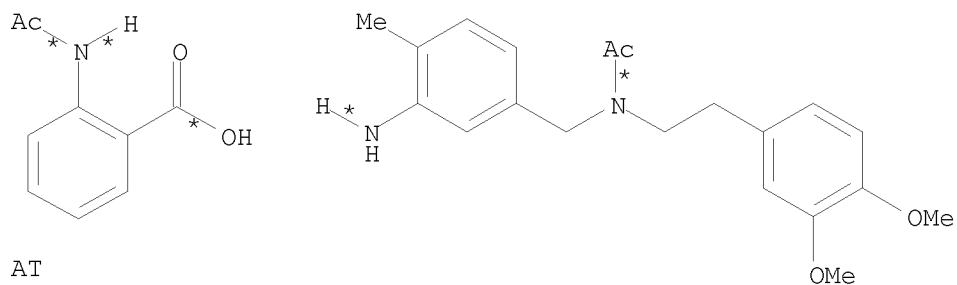
AU

RX(23) RCT AP 74101-71-6  
PRO AR 74101-73-8  
SOL 64-17-5 EtOH

RX(24) RCT AT 89-52-1, AR 74101-73-8  
PRO AU 74101-74-9  
CAT 538-75-0 DCC

RX(43) OF 58 COMPOSED OF RX(24), RX(27)

RX(43) AT + AR ==> AY

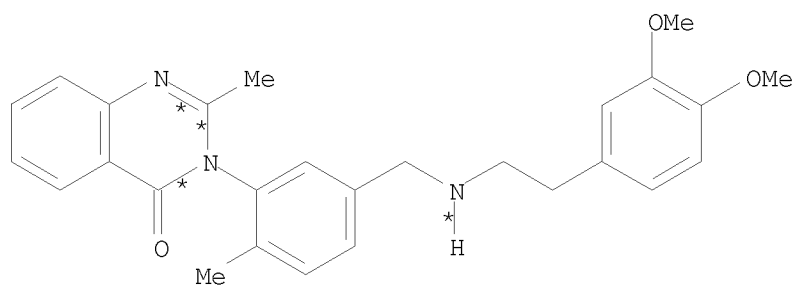


AT

AR

2  
STEPS  
→

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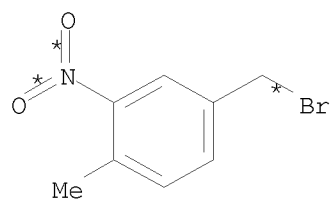


AY  
YIELD 16%

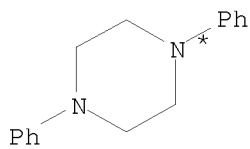
RX(24) RCT AT 89-52-1, AR 74101-73-8  
PRO AU 74101-74-9  
CAT 538-75-0 DCC

RX(27) RCT AU 74101-74-9  
RGT AZ 7647-01-0 HCl  
PRO AY 74101-76-1

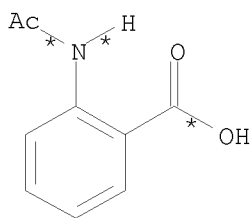
RX(48) OF 58 COMPOSED OF RX(19), RX(22), RX(25)  
RX(48) AJ + AL + AT ==> AW



AJ

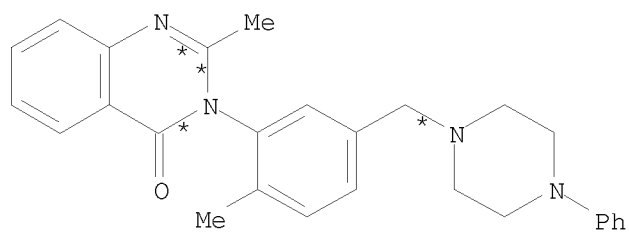


AL



AT

3  
STEPS  
→



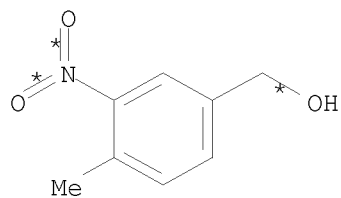
AW



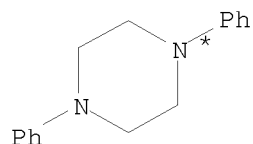
RX(19)      RCT    AJ 74101-68-1, AL 613-39-8  
              PRO    AM 74101-69-2

RX(22) RCT AM 74101-69-2  
PRO AQ 74101-72-7

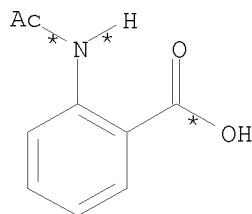
RX(25)      RCT    AT 89-52-1, AQ 74101-72-7  
               PRO    AW 74101-75-0  
               CAT    538-75-0 DCC

$$\begin{array}{lcl} \text{RX(49)} & \text{OF 58 COMPOSED OF RX(18), RX(19), RX(22), RX(25)} & \\ \text{RX(49)} & \text{AI + AL + AT} & \text{==> AW} \end{array}$$


AI

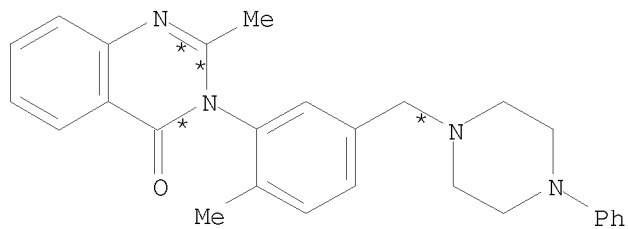


AL



AT

4  
STEPS



AW

RX(18)	RCT	AI	40870-59-5
	RGT	AK	7789-60-8 PBr3
	PRO	AJ	74101-68-1

RX(19)      RCT    AJ 74101-68-1, AL 613-39-8  
               PRO    AM 74101-69-2

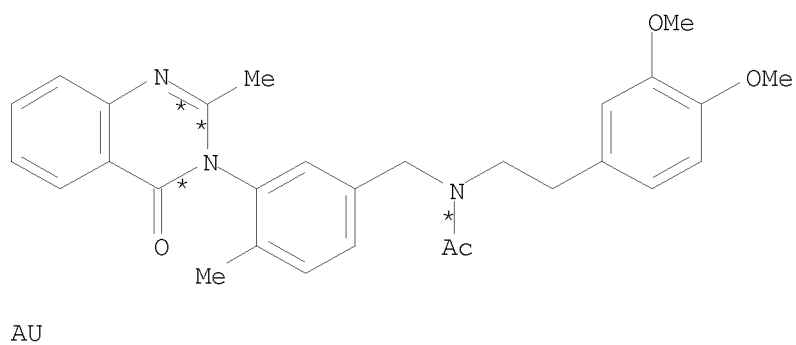
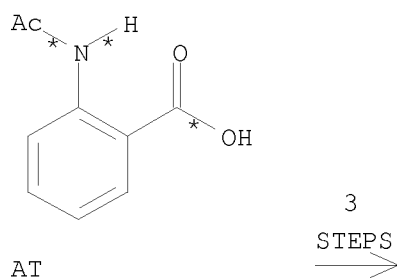
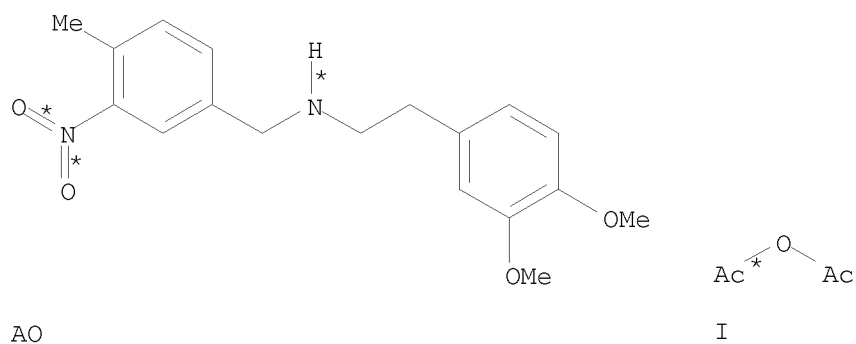
RX(22)	RCT	AM	74101-69-2
	PRO	AQ	74101-72-7

RX(25) RCT AT 89-52-1, AQ 74101-72-7

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PRO AW 74101-75-0  
CAT 538-75-0 DCC

RX(52) OF 58 COMPOSED OF RX(21), RX(23), RX(24)  
RX(52) AO + I + AT ==> AU



RX(21) RCT AO 74101-70-5, I 108-24-7  
PRO AP 74101-71-6

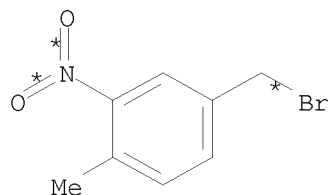
RX(23) RCT AP 74101-71-6  
PRO AR 74101-73-8  
SOL 64-17-5 EtOH

RX(24) RCT AT 89-52-1, AR 74101-73-8  
PRO AU 74101-74-9

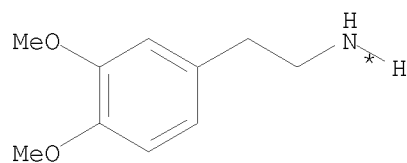
10/ 562,112

CAT 538-75-0 DCC

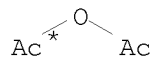
RX(53) OF 58 COMPOSED OF RX(20), RX(21), RX(23), RX(24)  
RX(53) AJ + AN + I + AT ==> AU



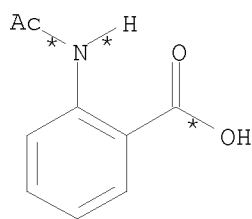
AJ



AN

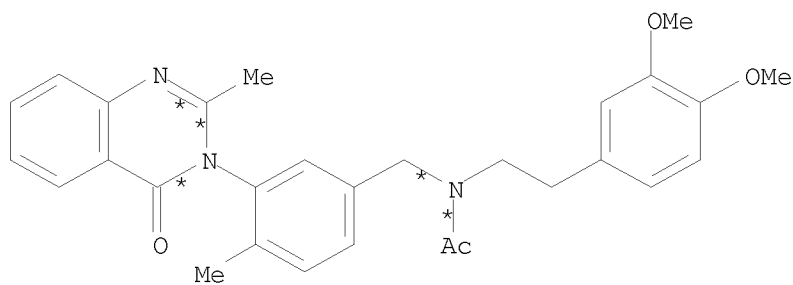


I



AT

4  
STEPS  
→



AU

RX(20) RCT AJ 74101-68-1, AN 120-20-7  
PRO AO 74101-70-5

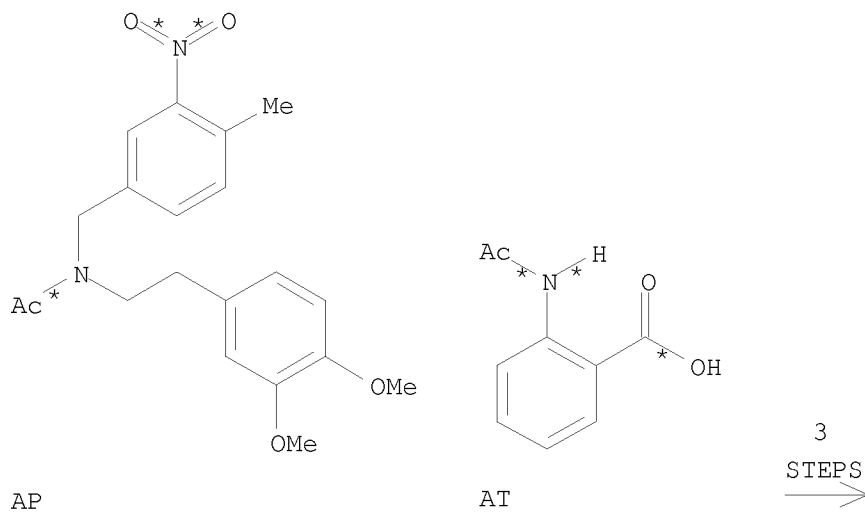
RX(21) RCT AO 74101-70-5, I 108-24-7  
PRO AP 74101-71-6

RX(23) RCT AP 74101-71-6  
PRO AR 74101-73-8  
SOL 64-17-5 EtOH

RX(24) RCT AT 89-52-1, AR 74101-73-8  
PRO AU 74101-74-9  
CAT 538-75-0 DCC

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RX(54) OF 58 COMPOSED OF RX(23), RX(24), RX(27)  
RX(54) AP + AT ==> AY



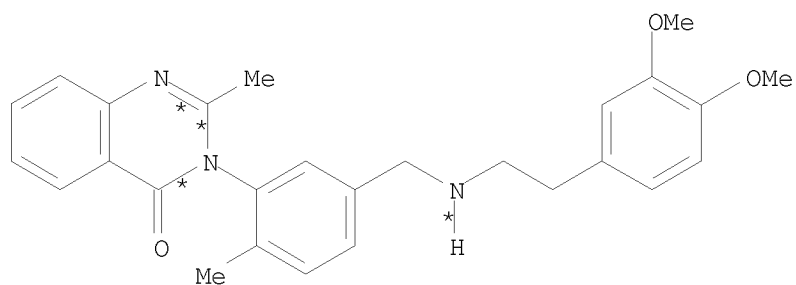
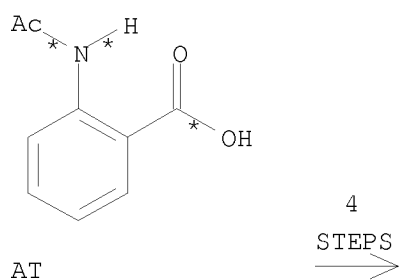
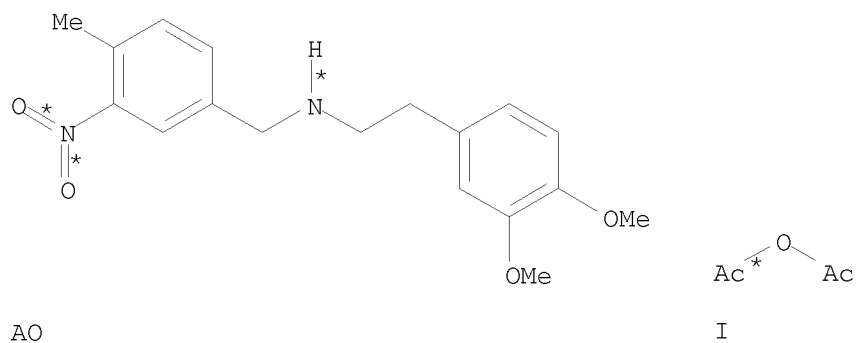
AY  
YIELD 16%

RX(23) RCT AP 74101-71-6  
PRO AR 74101-73-8  
SOL 64-17-5 EtOH

RX(24) RCT AT 89-52-1, AR 74101-73-8  
PRO AU 74101-74-9  
CAT 538-75-0 DCC

RX(27) RCT AU 74101-74-9  
RGT AZ 7647-01-0 HCl  
PRO AY 74101-76-1

RX(55) OF 58 COMPOSED OF RX(21), RX(23), RX(24), RX(27)  
RX(55) AO + I + AT ==> AY



AY  
YIELD 16%

RX(21) RCT AO 74101-70-5, I 108-24-7  
PRO AP 74101-71-6

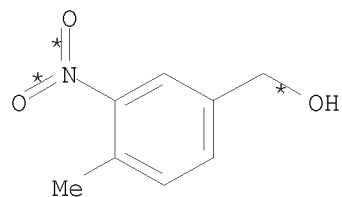
RX(23) RCT AP 74101-71-6  
PRO AR 74101-73-8  
SOL 64-17-5 EtOH

RX(24) RCT AT 89-52-1, AR 74101-73-8  
PRO AU 74101-74-9  
CAT 538-75-0 DCC

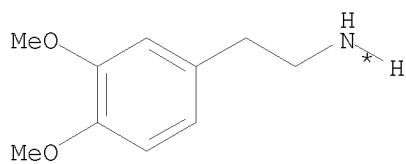
RX(27) RCT AU 74101-74-9  
RGT AZ 7647-01-0 HCl  
PRO AY 74101-76-1

10/ 562,112

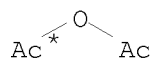
RX(56) OF 58 COMPOSED OF RX(18), RX(20), RX(21), RX(23), RX(24)  
RX(56) AI + AN + I + AT ==> AU



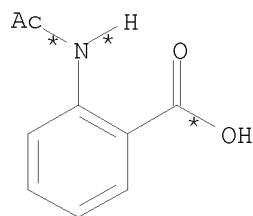
AI



AN

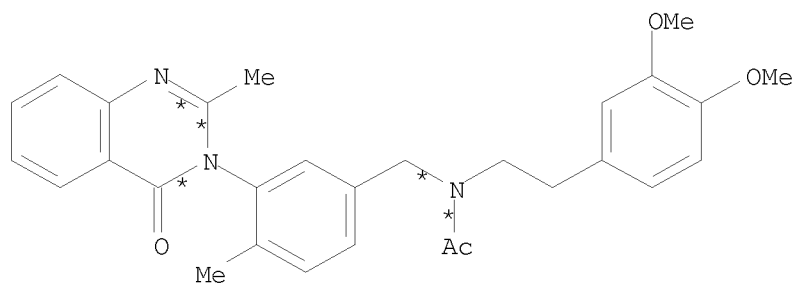


I



AT

5  
STEPS  
→



AU

RX(18) RCT AI 40870-59-5  
RGT AK 7789-60-8 PBr3  
PRO AJ 74101-68-1

RX(20) RCT AJ 74101-68-1, AN 120-20-7  
PRO AO 74101-70-5

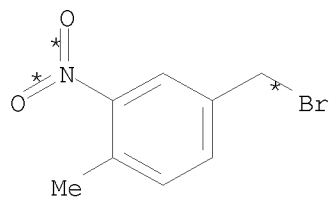
RX(21) RCT AO 74101-70-5, I 108-24-7  
PRO AP 74101-71-6

RX(23) RCT AP 74101-71-6  
PRO AR 74101-73-8  
SOL 64-17-5 EtOH

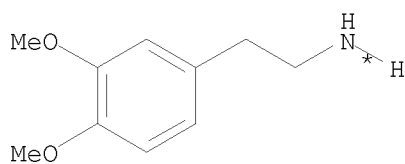
10/ 562,112

RX(24) RCT AT 89-52-1, AR 74101-73-8  
PRO AU 74101-74-9  
CAT 538-75-0 DCC

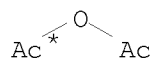
RX(57) OF 58 COMPOSED OF RX(20), RX(21), RX(23), RX(24), RX(27)  
RX(57) AJ + AN + I + AT ==> AY



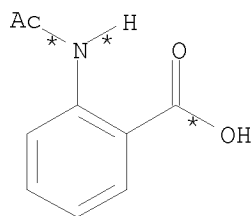
AJ



AN

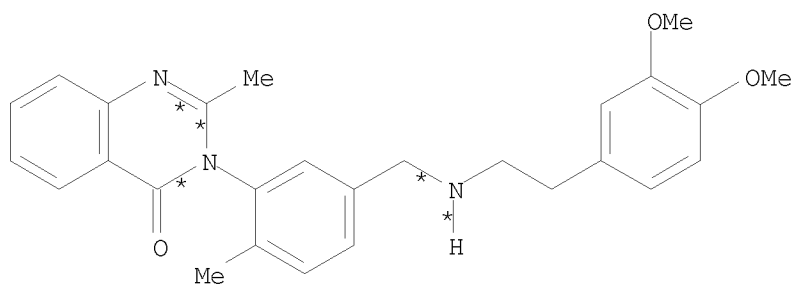


I



AT

5  
STEPS  
→



AY  
YIELD 16%

RX(20) RCT AJ 74101-68-1, AN 120-20-7  
PRO AO 74101-70-5

RX(21) RCT AO 74101-70-5, I 108-24-7  
PRO AP 74101-71-6

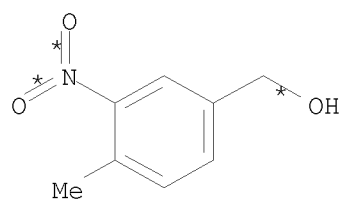
RX(23) RCT AP 74101-71-6  
PRO AR 74101-73-8  
SOL 64-17-5 EtOH

10/ 562,112

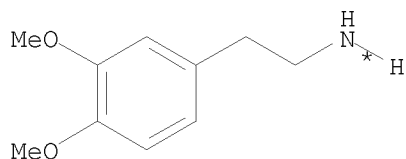
RX(24) RCT AT 89-52-1, AR 74101-73-8  
PRO AU 74101-74-9  
CAT 538-75-0 DCC

RX(27) RCT AU 74101-74-9  
RGT AZ 7647-01-0 HCl  
PRO AY 74101-76-1

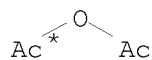
RX(58) OF 58 COMPOSED OF RX(18), RX(20), RX(21), RX(23), RX(24), RX(27)  
RX(58) AI + AN + I + AT ==> AY



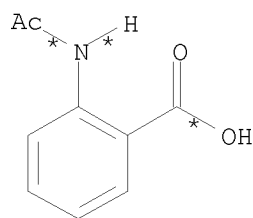
AI



AN

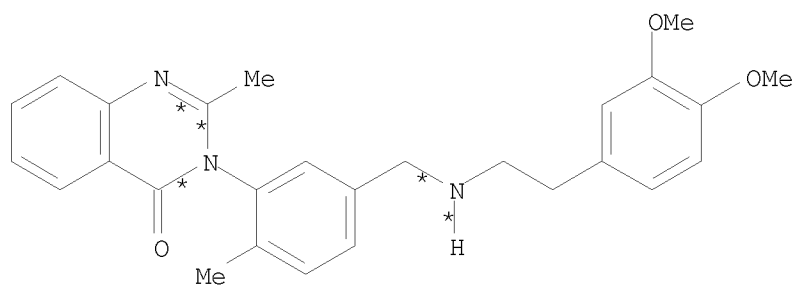


I



AT

6  
STEPS  
→



AY  
YIELD 16%

RX(18) RCT AI 40870-59-5  
RGT AK 7789-60-8 PBr3  
PRO AJ 74101-68-1

RX(20) RCT AJ 74101-68-1, AN 120-20-7  
PRO AO 74101-70-5



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RX(21) RCT AO 74101-70-5, I 108-24-7  
PRO AP 74101-71-6

RX(23) RCT AP 74101-71-6  
PRO AR 74101-73-8  
SOL 64-17-5 EtOH

RX(24) RCT AT 89-52-1, AR 74101-73-8  
PRO AU 74101-74-9  
CAT 538-75-0 DCC

RX(27) RCT AU 74101-74-9  
RGT AZ 7647-01-0 HCl  
PRO AY 74101-76-1

L3 ANSWER 230 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 93:26374 CASREACT

TITLE: Studies on biologically active halogenated compounds.  
II. Chemical modifications of

AUTHOR(S):

6-amino-2-fluoromethyl-3-[o-tolyl]-4[3H]-quinazolinone  
and the CNS depressant activities of related compounds  
Tani, Junichi; Yamada, Yoshihisa; Ochiai, Takashi;  
Ishida, Ryuichi; Inoue, Ichizo; Oine, Toyonari

CORPORATE SOURCE:

Res. Lab., Tanabe Seiyaku Co., Ltd., Osaka, 532, Japan  
Chemical & Pharmaceutical Bulletin (1979), 27(11),  
2675-87

SOURCE:

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE:

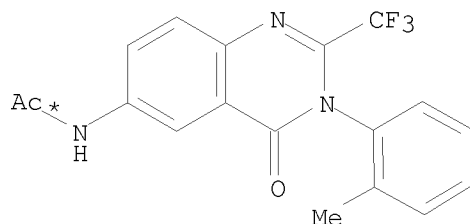
Journal

LANGUAGE:

English

AB A number of derivs. of 6-amino-2-fluoromethyl-3-(o-tolyl)-4(3H)-quinazolinone (6-aminomethaqualone), a potent muscle relaxant, were prepared and screened in terms of the loss of righting reflex test and the rotating rod test in mice. Several derivs. with addnl. F substitution or with repositioning of the F atom exhibited high activities. Other structural modification included acylation, carbamoylation, and alkoxycarbonylation of the 6-amino group, hydroxylation at the 3-tolyl group, and replacement of the F atom at the 2-fluoromethyl group by O, N and S nucleophiles; these modification all resulted in loss of activity.

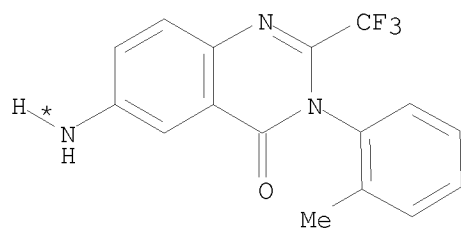
RX(2) OF 91 ...D ==> E



D



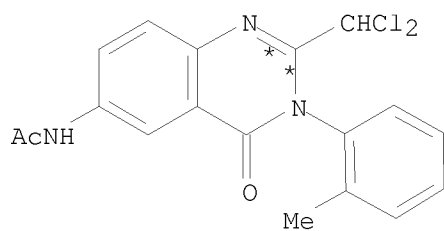
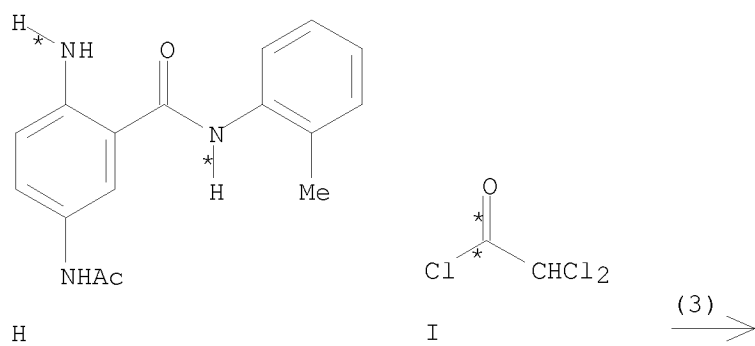
10/ 562,112



E

RX(2)      RCT   D 73832-50-5  
             RGT   F 7647-01-0 HCl  
             PRO   E 73832-08-3  
             SOL   67-56-1 MeOH

RX(3) OF 91      H   +   I   ==>   J

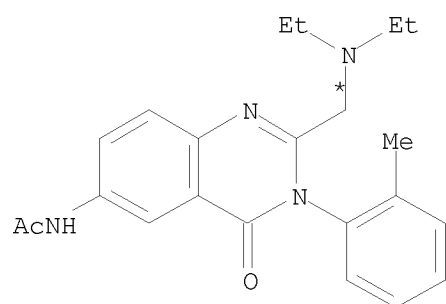
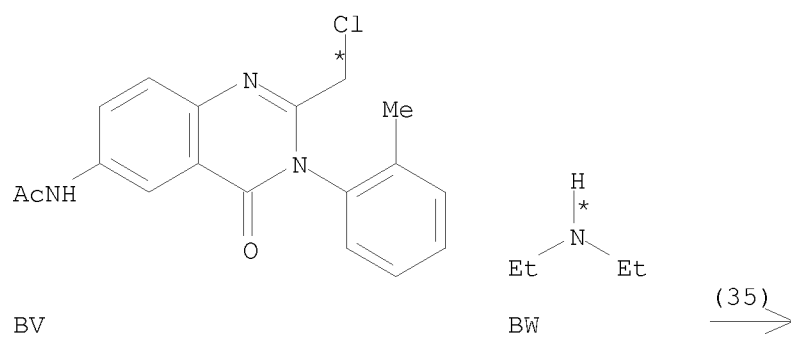


J

RX(3)      RCT   H 64102-81-4, I 79-36-7  
             RGT   K 7637-07-2 BF<sub>3</sub>  
             PRO   J 73832-51-6  
             SOL   60-29-7 Et<sub>2</sub>O

RX(35) OF 91      BV   +   BW   ==>   BX...

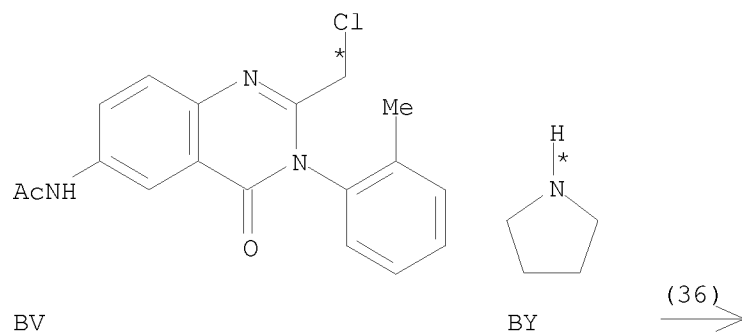
10/ 562,112



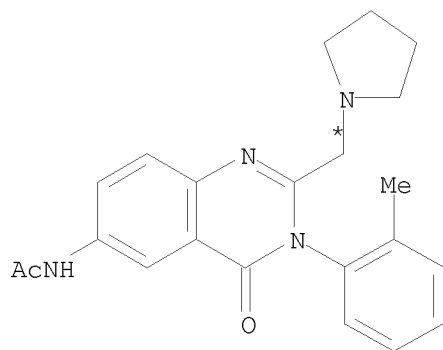
BX

RX(35)      RCT    BV 61899-78-3, BW 109-89-7  
              PRO    BX 73832-71-0  
              SOL    109-99-9 THF

RX(36) OF 91      BV + BY ==> BZ



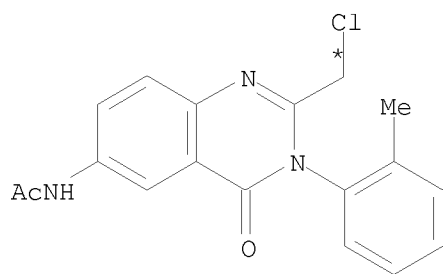
10/ 562,112



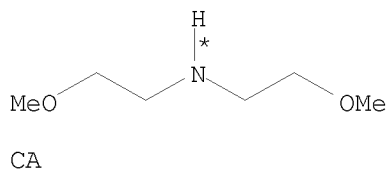
BZ

RX(36)      RCT    BV 61899-78-3, BY 123-75-1  
              PRO    BZ 73832-81-2  
              SOL    109-99-9 THF

RX(37) OF 91      BV    +    CA    ==>    CB...

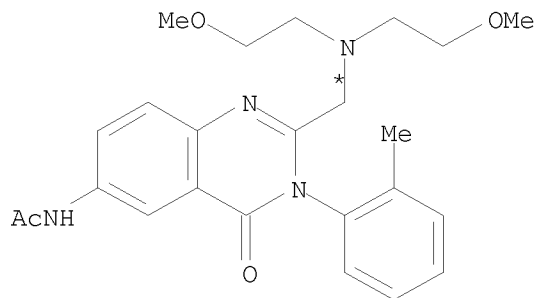


BV



CA

(37)  
→



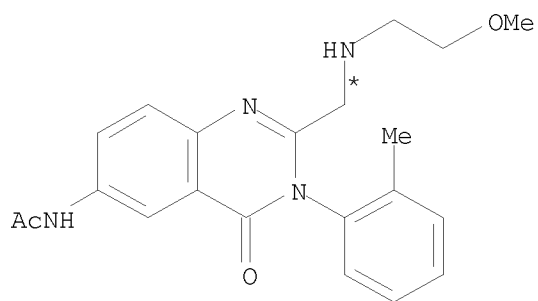
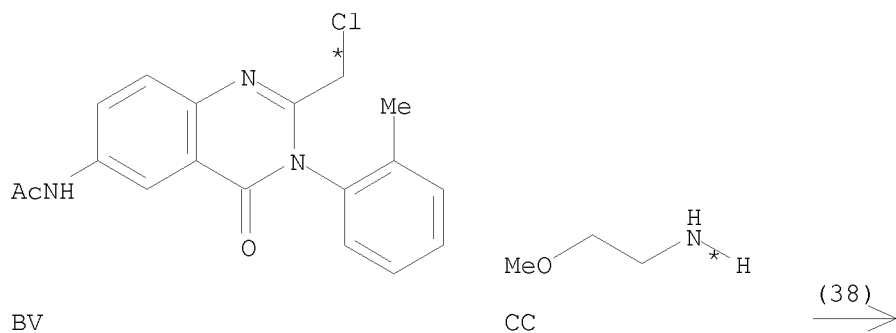
CB

RX(37)      RCT    BV 61899-78-3, CA 111-95-5  
              PRO    CB 73832-82-3

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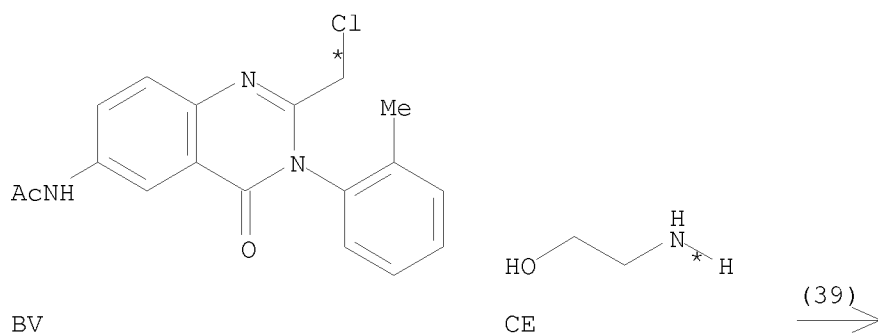
SOL 109-99-9 THF

RX(38) OF 91 BV + CC ==> CD...

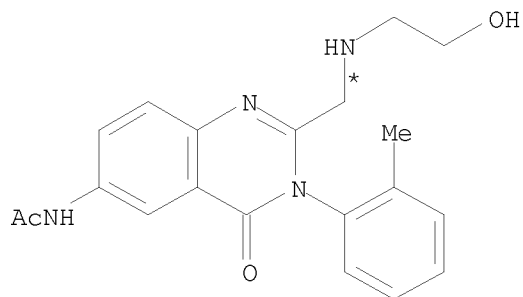


RX(38) RCT BV 61899-78-3, CC 109-85-3  
PRO CD 73832-84-5  
SOL 109-99-9 THF

RX(39) OF 91 BV + CE ==> CF...



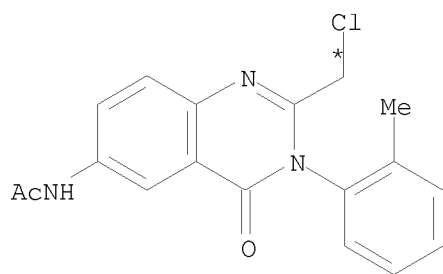
10/ 562,112



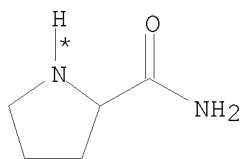
CF

RX(39)      RCT    BV 61899-78-3, CE 141-43-5  
              PRO    CF 73832-85-6  
              SOL    109-99-9 THF

RX(40) OF 91      BV   +   CG   ==>   CH...

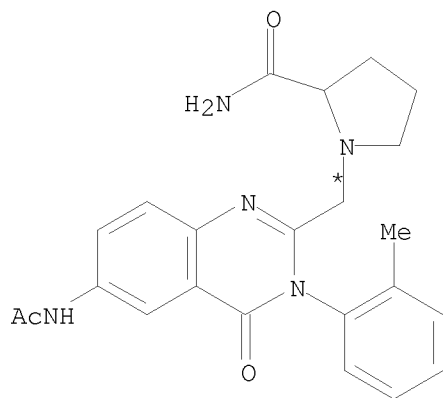


BV



CG

(40)

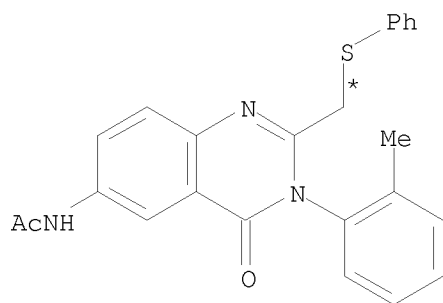
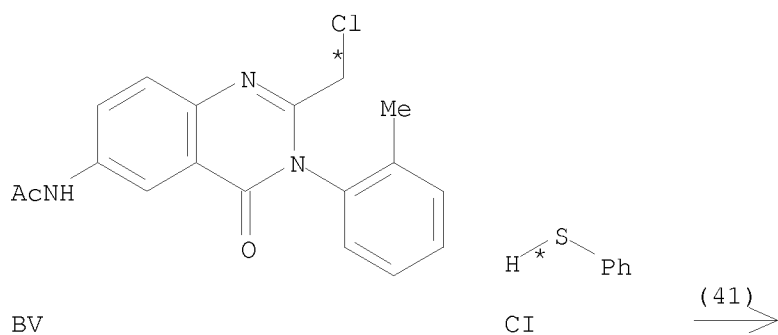


CH

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RX(40)      RCT    BV 61899-78-3, CG 2812-47-7  
             PRO    CH 73832-87-8  
             SOL    109-99-9 THF

RX(41) OF 91      BV + CI ==> CJ...

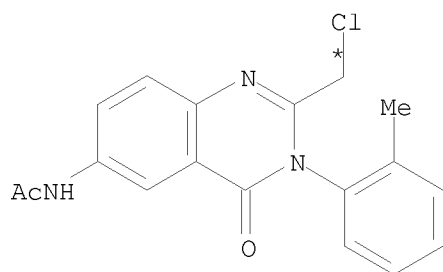


CJ

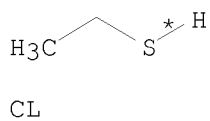
RX(41)      RCT    BV 61899-78-3, CI 108-98-5  
             RGT    CK 7646-69-7 NaH  
             PRO    CJ 73832-73-2  
             SOL    109-99-9 THF

RX(42) OF 91      BV + CL ==> CM...

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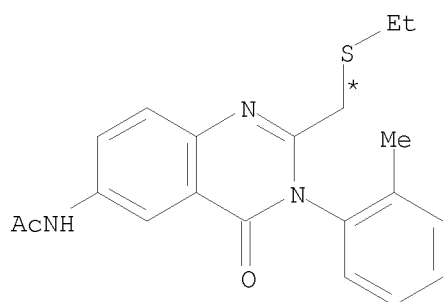


BV



CL

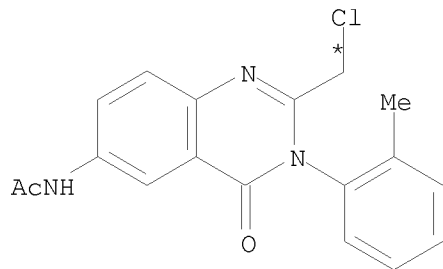
(42)



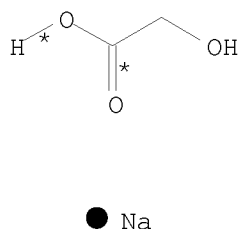
CM

RX(42)     RCT    BV 61899-78-3, CL 75-08-1  
              RGT    CK 7646-69-7 NaH  
              PRO    CM 73832-88-9  
              SOL    109-99-9 THF

RX(43) OF 91     BV + CN ==> CO...



BV



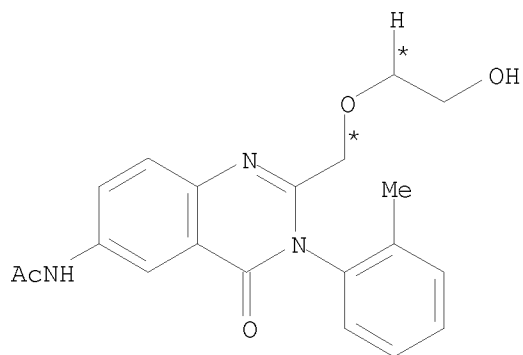
CN

● Na

(43)



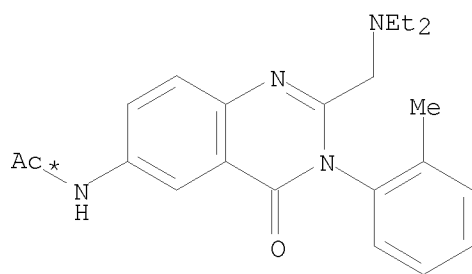
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CO

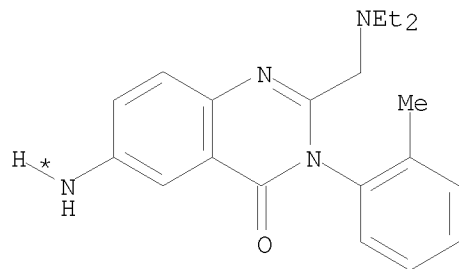
RX(43) RCT BV 61899-78-3, CN 2836-32-0  
PRO CO 73832-89-0

RX(44) OF 91 ...BX ==> CP



BX

(44)  
→



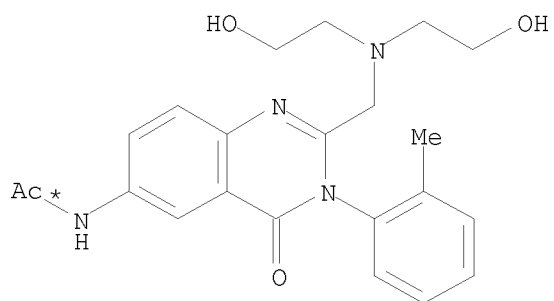
CP

RX(44) RCT BX 73832-71-0  
RGT F 7647-01-0 HCl  
PRO CP 73832-37-8

10/ 562,112

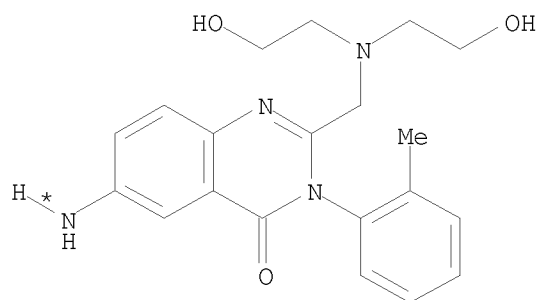
SOL 67-56-1 MeOH

RX(45) OF 91 ...CQ ==> CR



CQ

(45)

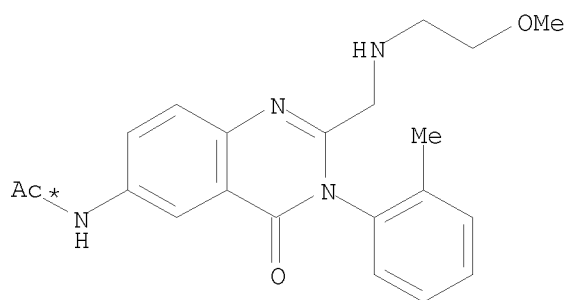


CR

RX(45) RCT CQ 73832-83-4  
RGT F 7647-01-0 HCl  
PRO CR 73832-41-4  
SOL 67-56-1 MeOH

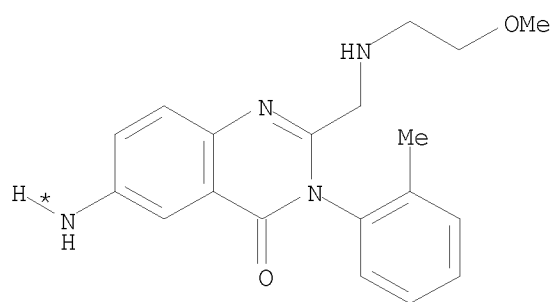
RX(46) OF 91 ...CD ==> CS

10/ 562,112



CD

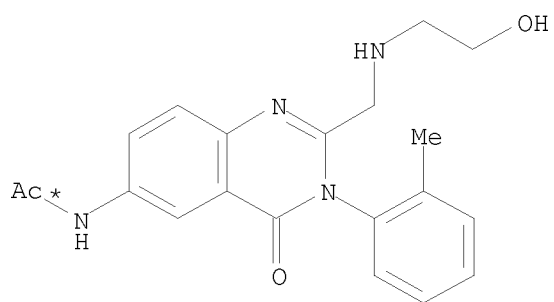
(46)  $\longrightarrow$



CS

RX(46)      RCT    CD 73832-84-5  
              RGT    F 7647-01-0 HCl  
              PRO    CS 73832-42-5  
              SOL    67-56-1 MeOH

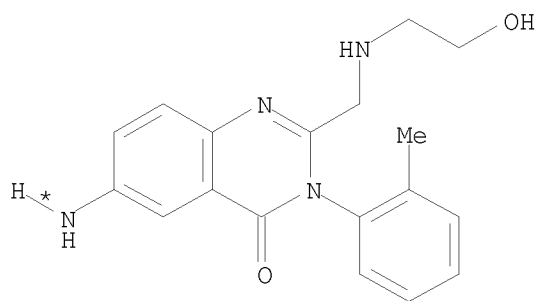
RX(47) OF 91      ...CF    ==>    CT



CF

(47)  $\longrightarrow$

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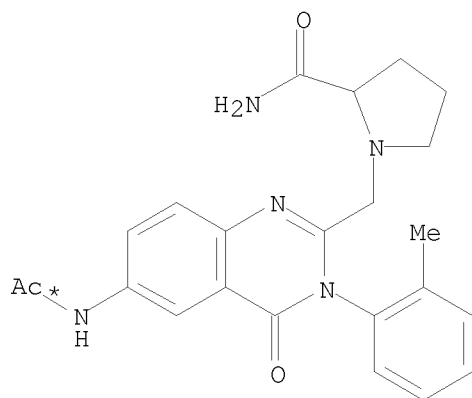


● 2 HCl

CT

RX(47)      RCT    CF 73832-85-6  
              RGT    F 7647-01-0 HCl  
              PRO    CT 73832-43-6  
              SOL    67-56-1 MeOH

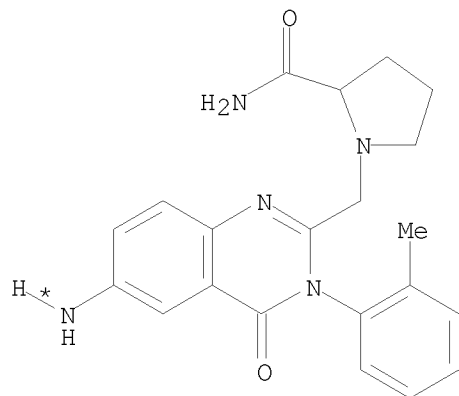
RX(48) OF 91      ...CH ==> CU



CH

(48)

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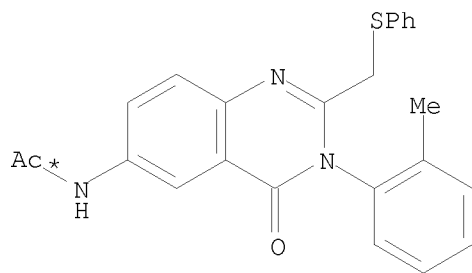


● 2 HCl

CU

RX(48)     RCT   CH 73832-87-8  
             RGT   F 7647-01-0 HCl  
             PRO   CU 73832-45-8  
             SOL   67-56-1 MeOH

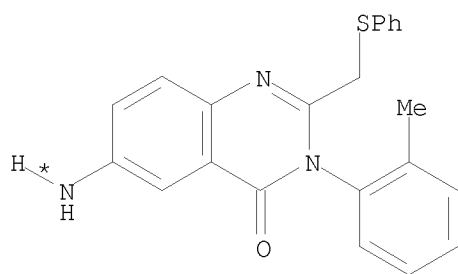
RX(49) OF 91     ...CJ   ==>   CV



CJ

(49) 

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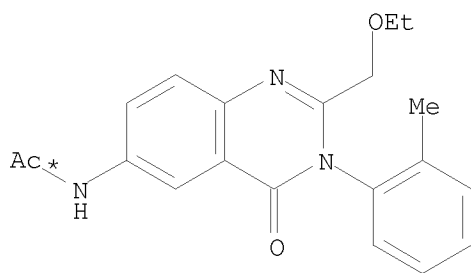


● HCl

CV

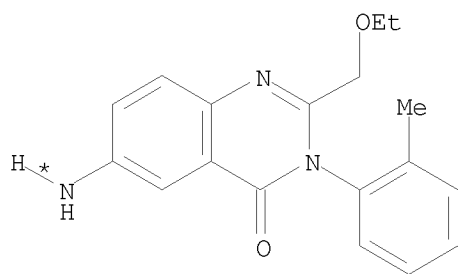
RX(49)      RCT    CJ 73832-73-2  
              RGT    F 7647-01-0 HCl  
              PRO    CV 73832-46-9  
              SOL    67-56-1 MeOH

RX(50) OF 91      ...CW ==> CX



CW

(50)

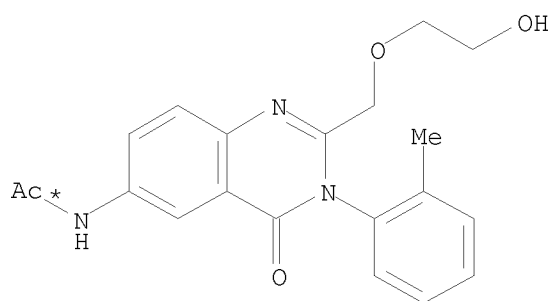


CX

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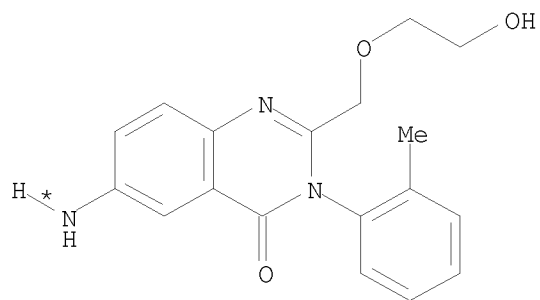
RX(50)      RCT    CW 73832-72-1  
              RGT    F 7647-01-0 HCl  
              PRO    CX 73832-48-1  
              SOL    67-56-1 MeOH

RX(51) OF 91      ...CO    ==>    CY



CO

(51)  
→

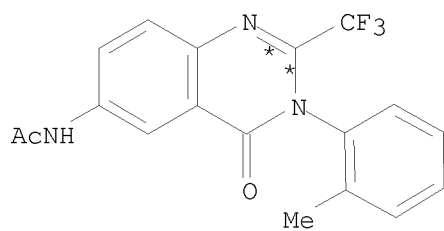
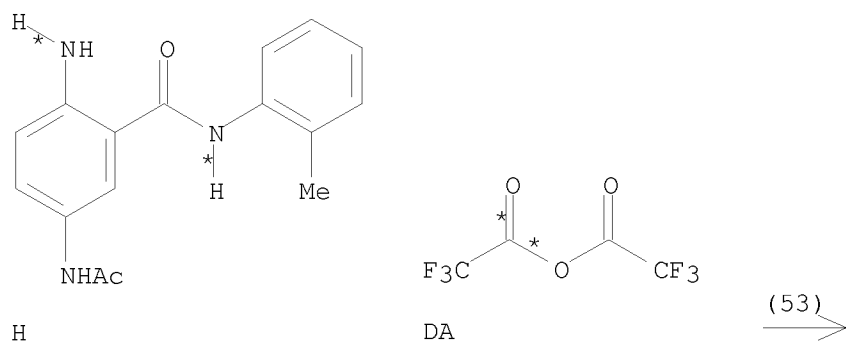


CY

RX(51)      RCT    CO 73832-89-0  
              RGT    F 7647-01-0 HCl  
              PRO    CY 73832-90-3  
              SOL    67-56-1 MeOH

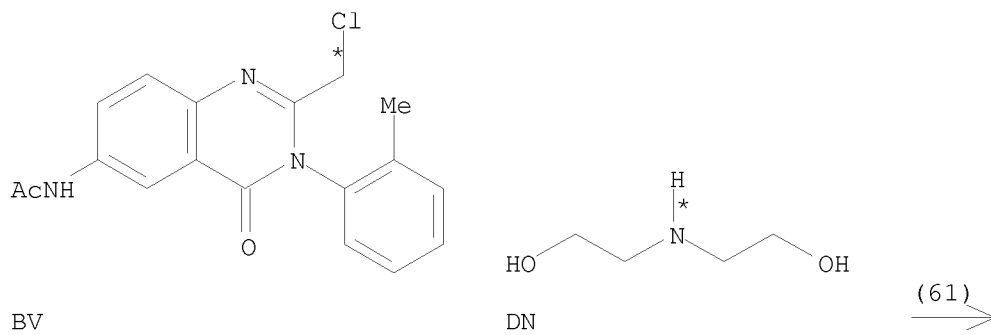
RX(53) OF 91      H    +    DA    ==>    D...

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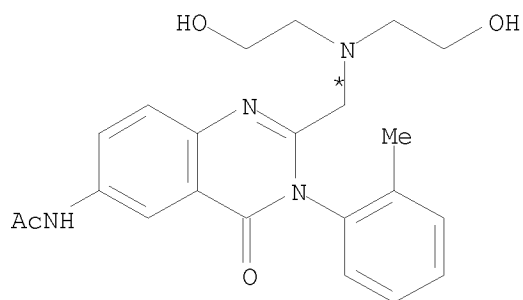
RX(53)      RCT    H 64102-81-4, DA 407-25-0  
               RGT    K 7637-07-2 BF3  
               PRO    D 73832-50-5  
               SOL    407-25-0 (CF3CO)2O, 60-29-7 Et2O

RX(61) OF 91      BV + DN ==> CQ...





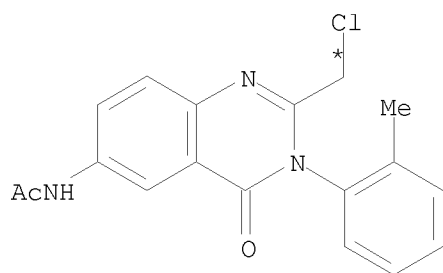
10/ 562,112



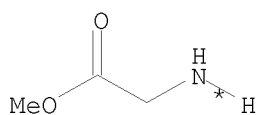
CQ

RX(61) RCT BV 61899-78-3, DN 111-42-2  
PRO CQ 73832-83-4  
SOL 109-99-9 THF

RX(62) OF 91 BV + DO ==> DP...

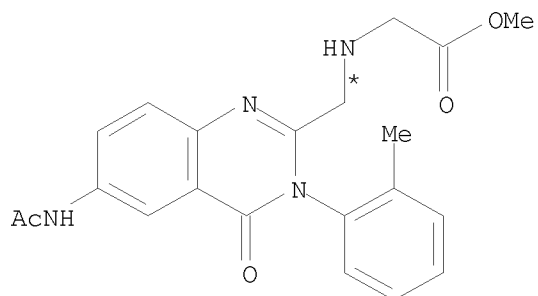


BV



DO

(62)  $\longrightarrow$

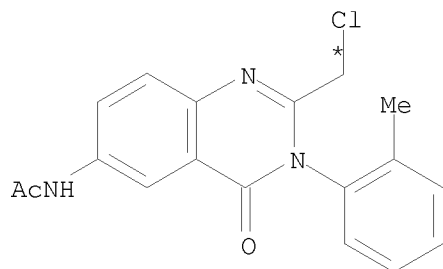


DP

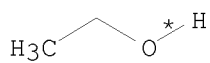
RX(62) RCT BV 61899-78-3, DO 616-34-2  
PRO DP 73832-86-7  
SOL 109-99-9 THF

10/ 562,112

RX(63) OF 91 BV + DQ ==> CW...

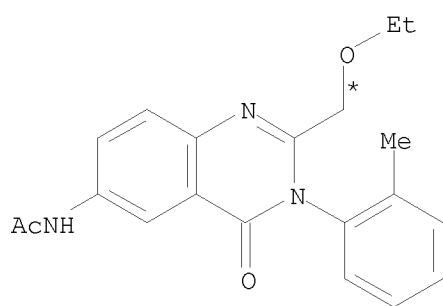


BV



DQ

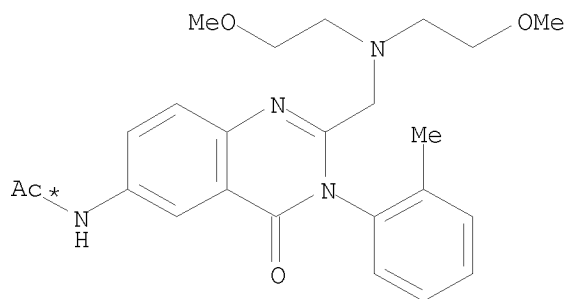
(63)



CW

RX(63) RCT BV 61899-78-3, DQ 141-52-6  
 PRO CW 73832-72-1  
 SOL 64-17-5 EtOH

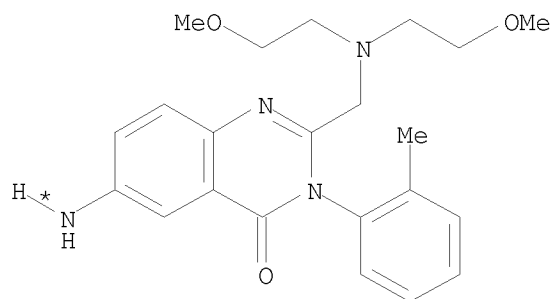
RX(64) OF 91 ...CB ==> DS



CB

(64)

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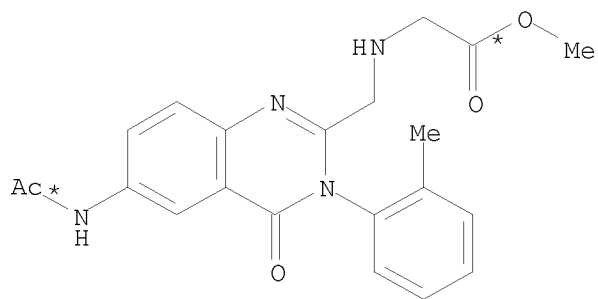


●2 HCl

DS

RX(64)      RCT    CB 73832-82-3  
              RGT    F 7647-01-0 HCl  
              PRO    DS 73832-40-3  
              SOL    67-56-1 MeOH

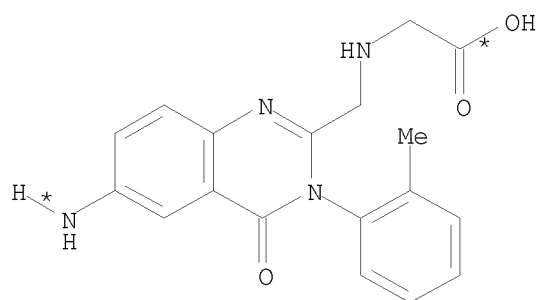
RX(65) OF 91      ...DP ==> DT



DP

(65) →

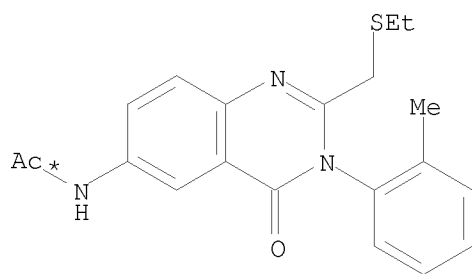
10/ 562,112



DT

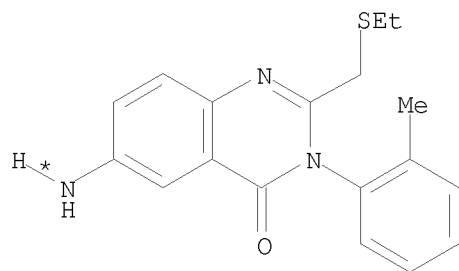
RX(65)      RCT    DP 73832-86-7  
                  RGT    F 7647-01-0 HCl  
                  PRO    DT 73832-44-7  
                  SOL    67-56-1 MeOH

RX(66) OF 91      ...CM    ==>    DU



CM

(66)  
 →



● HCl

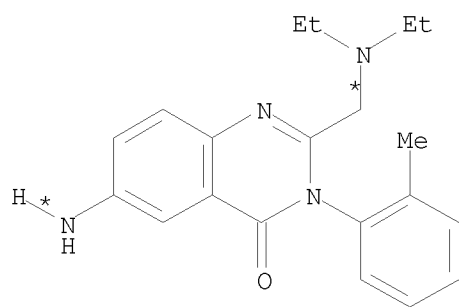
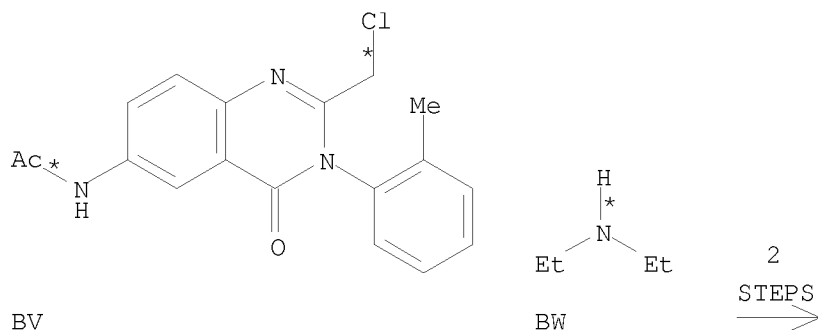
DU

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RX(66)      RCT    CM 73832-88-9  
              RGT    F 7647-01-0 HCl  
              PRO    DU 73832-47-0  
              SOL    67-56-1 MeOH

RX(77) OF 91 COMPOSED OF RX(35), RX(44)

RX(77)      BV + BW ==> CP



CP

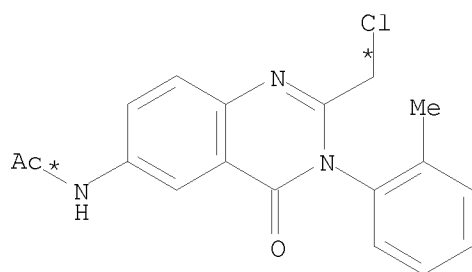
RX(35)      RCT    BV 61899-78-3, BW 109-89-7  
              PRO    BX 73832-71-0  
              SOL    109-99-9 THF

RX(44)      RCT    BX 73832-71-0  
              RGT    F 7647-01-0 HCl  
              PRO    CP 73832-37-8  
              SOL    67-56-1 MeOH

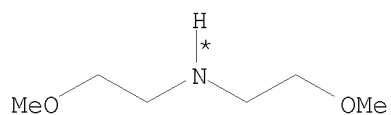
RX(78) OF 91 COMPOSED OF RX(37), RX(64)

RX(78)      BV + CA ==> DS

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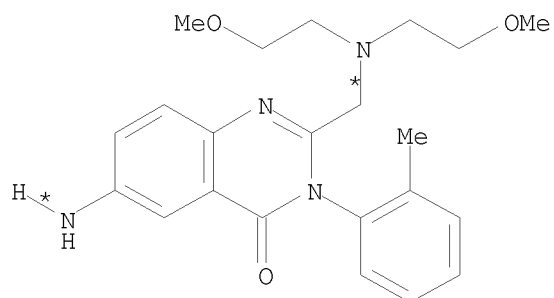


BV



CA

2  
STEPS  
→



● 2 HCl

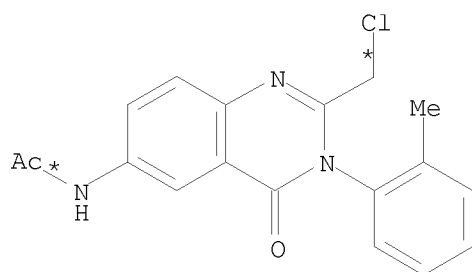
DS

RX(37) RCT BV 61899-78-3, CA 111-95-5  
PRO CB 73832-82-3  
SOL 109-99-9 THF

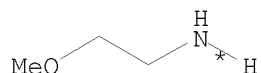
RX(64) RCT CB 73832-82-3  
RGT F 7647-01-0 HCl  
PRO DS 73832-40-3  
SOL 67-56-1 MeOH

RX(79) OF 91 COMPOSED OF RX(38), RX(46)  
RX(79) BV + CC ==> CS

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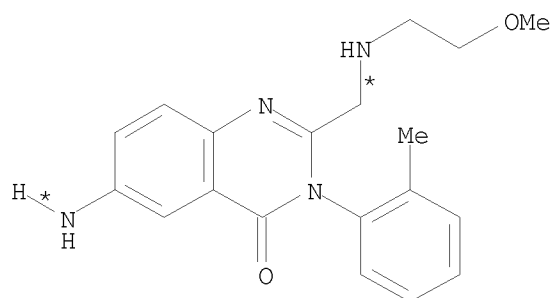


BV



CC

2  
STEPS  
→



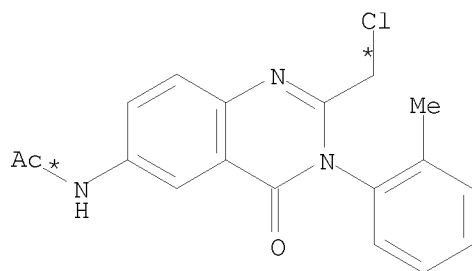
CS

RX(38)     RCT    BV 61899-78-3, CC 109-85-3  
             PRO    CD 73832-84-5  
             SOL    109-99-9 THF

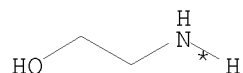
RX(46)     RCT    CD 73832-84-5  
             RGT    F 7647-01-0 HCl  
             PRO    CS 73832-42-5  
             SOL    67-56-1 MeOH

RX(80) OF 91 COMPOSED OF RX(39), RX(47)

RX(80)     BV + CE ==> CT



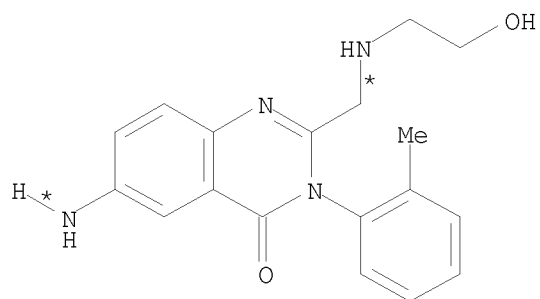
BV



CE

2  
STEPS  
→

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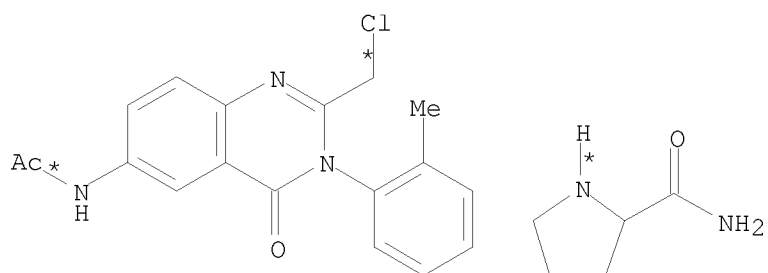
● 2 HCl

CT

RX(39) RCT BV 61899-78-3, CE 141-43-5  
PRO CF 73832-85-6  
SOL 109-99-9 THF

RX(47) RCT CF 73832-85-6  
RGT F 7647-01-0 HCl  
PRO CT 73832-43-6  
SOL 67-56-1 MeOH

RX(81) OF 91 COMPOSED OF RX(40), RX(48)  
RX(81) BV + CG ==> CU



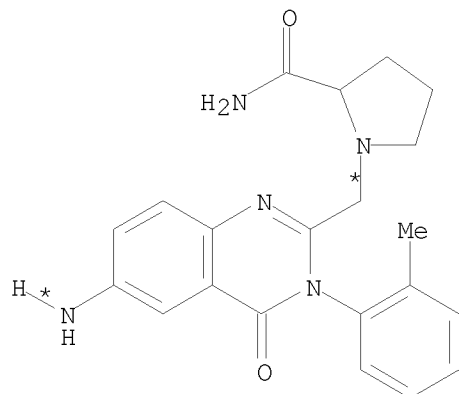
BV

CG

2  
STEPS  
→



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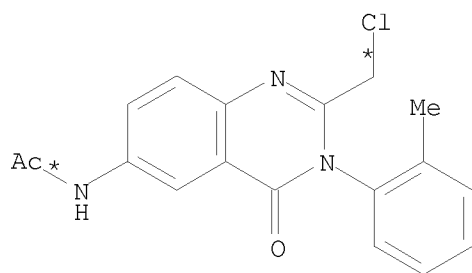
● 2 HCl

CU

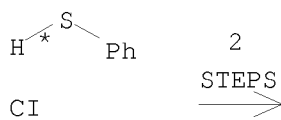
RX(40) RCT BV 61899-78-3, CG 2812-47-7  
PRO CH 73832-87-8  
SOL 109-99-9 THF

RX(48) RCT CH 73832-87-8  
RGT F 7647-01-0 HCl  
PRO CU 73832-45-8  
SOL 67-56-1 MeOH

RX(82) OF 91 COMPOSED OF RX(41), RX(49)  
RX(82) BV + CI ==> CV

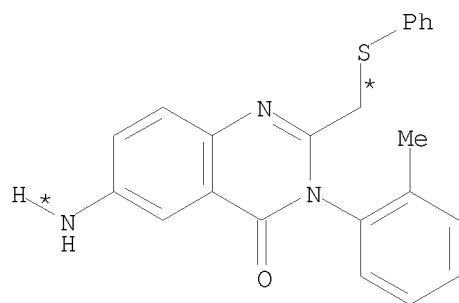


BV



2  
STEPS  
→

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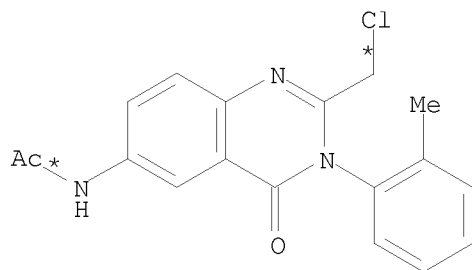
● HCl

CV

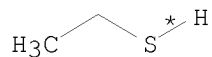
RX(41) RCT BV 61899-78-3, CI 108-98-5  
RGT CK 7646-69-7 NaH  
PRO CJ 73832-73-2  
SOL 109-99-9 THF

RX(49) RCT CJ 73832-73-2  
RGT F 7647-01-0 HCl  
PRO CV 73832-46-9  
SOL 67-56-1 MeOH

RX(83) OF 91 COMPOSED OF RX(42), RX(66)  
RX(83) BV + CL ==> DU



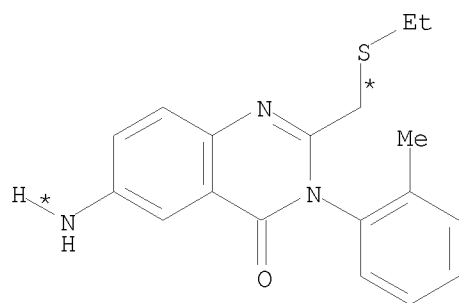
BV



CL

2  
STEPS  
→

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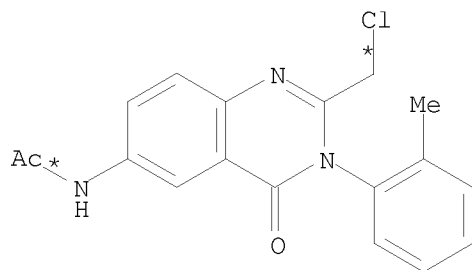
● HCl

DU

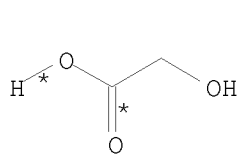
RX(42)     RCT    BV 61899-78-3, CL 75-08-1  
             RGT    CK 7646-69-7 NaH  
             PRO    CM 73832-88-9  
             SOL    109-99-9 THF

RX(66)     RCT    CM 73832-88-9  
             RGT    F 7647-01-0 HCl  
             PRO    DU 73832-47-0  
             SOL    67-56-1 MeOH

RX(84) OF 91 COMPOSED OF RX(43), RX(51)  
RX(84)     BV + CN ==> CY



BV

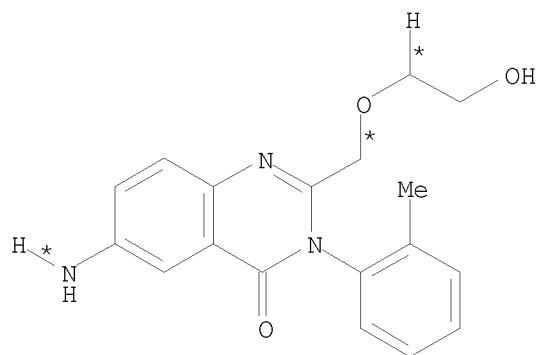


● Na

CN

2  
STEPS  
→

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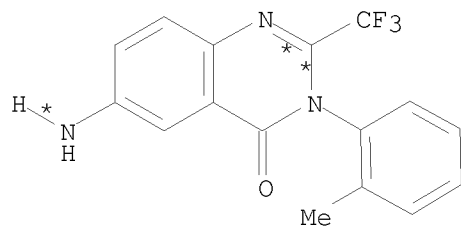
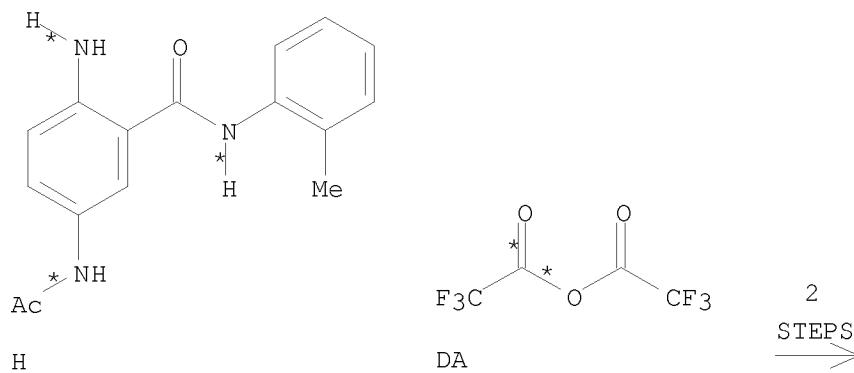


CY

RX(43) RCT BV 61899-78-3, CN 2836-32-0  
PRO CO 73832-89-0

RX(51) RCT CO 73832-89-0  
RGT F 7647-01-0 HCl  
PRO CY 73832-90-3  
SOL 67-56-1 MeOH

RX(85) OF 91 COMPOSED OF RX(53), RX(2)  
RX(85) H + DA ==> E



E

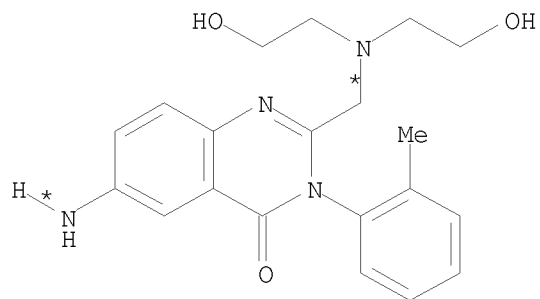
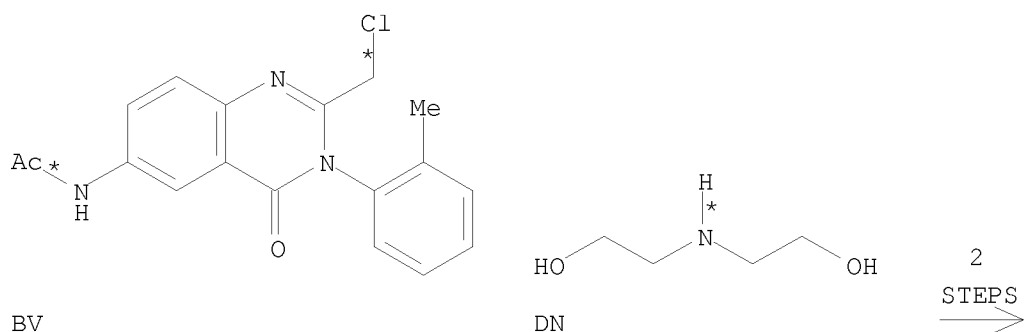
10/ 562,112

RX(53) RCT H 64102-81-4, DA 407-25-0  
RGT K 7637-07-2 BF3  
PRO D 73832-50-5  
SOL 407-25-0 (CF3CO)2O, 60-29-7 Et2O

RX(2) RCT D 73832-50-5  
RGT F 7647-01-0 HCl  
PRO E 73832-08-3  
SOL 67-56-1 MeOH

RX(88) OF 91 COMPOSED OF RX(61), RX(45)

RX(88) BV + DN ==> CR



CR

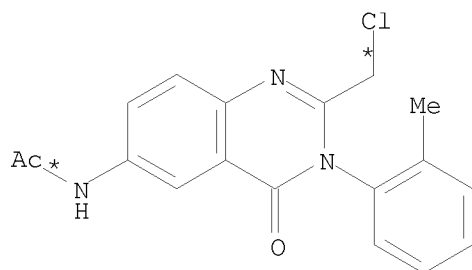
RX(61) RCT BV 61899-78-3, DN 111-42-2  
PRO CQ 73832-83-4  
SOL 109-99-9 THF

RX(45) RCT CQ 73832-83-4  
RGT F 7647-01-0 HCl  
PRO CR 73832-41-4  
SOL 67-56-1 MeOH

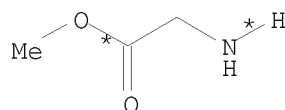
RX(89) OF 91 COMPOSED OF RX(62), RX(65)

RX(89) BV + DO ==> DT

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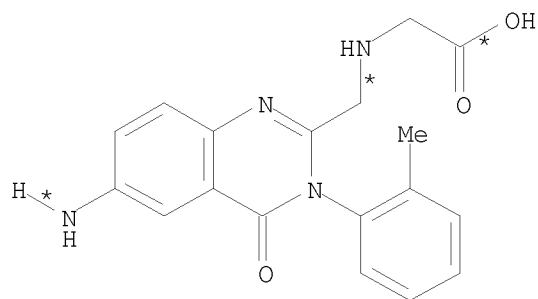


BV



DO

2  
STEPS  
→



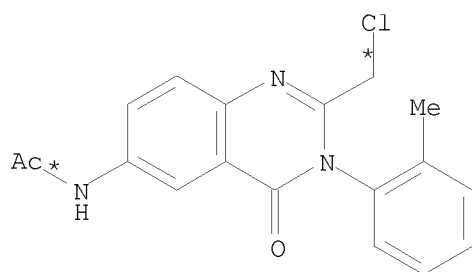
DT

RX(62)      RCT    BV 61899-78-3, DO 616-34-2  
             PRO    DP 73832-86-7  
             SOL    109-99-9 THF

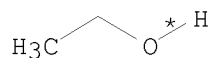
RX(65)      RCT    DP 73832-86-7  
             RGT    F 7647-01-0 HCl  
             PRO    DT 73832-44-7  
             SOL    67-56-1 MeOH

RX(90) OF 91 COMPOSED OF RX(63), RX(50)

RX(90)      BV + DQ ==> CX



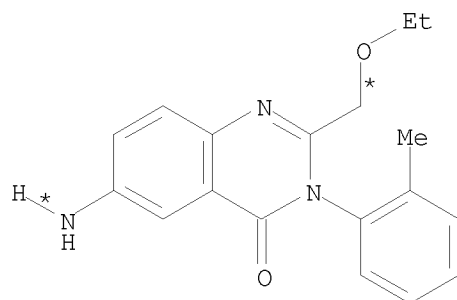
BV



DQ



2  
STEPS  
→



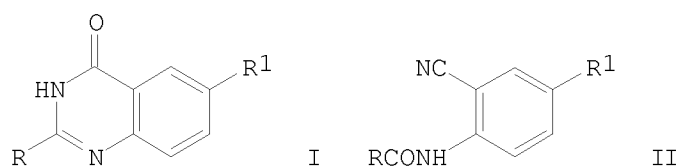
CX

RX(63)      RCT    BV 61899-78-3, DQ 141-52-6  
               PRO    CW 73832-72-1  
               SOL    64-17-5 EtOH

RX(50)      RCT    CW 73832-72-1  
               RGT    F 7647-01-0 HCl  
               PRO    CX 73832-48-1  
               SOL    67-56-1 MeOH

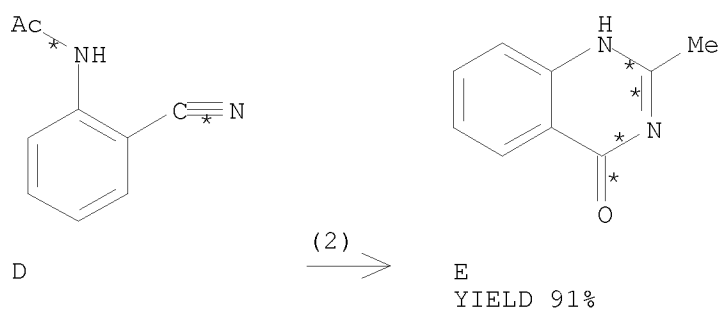
L3    ANSWER 231 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER:        93:8126    CASREACT  
 TITLE:                      A facile synthesis of  
                                  2-substituted-4(3H)-quinazolinones  
 AUTHOR(S):                Showell, Graham A.  
 CORPORATE SOURCE:        Med. Res. Cent., Beecham Pharm., Harlow/Essex, CM19  
                                  5AD, UK  
 SOURCE:                    Synthetic Communications (1980), 10(3), 241-3  
                                  CODEN: SYNCAV; ISSN: 0039-7911  
 DOCUMENT TYPE:            Journal  
 LANGUAGE:                 English  
 GI

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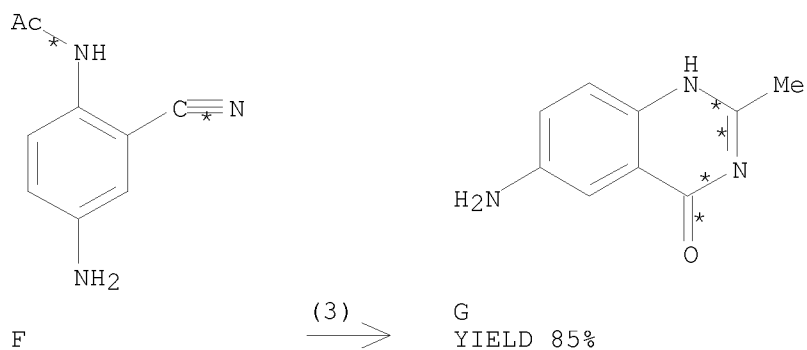
AB    Quinazolones I (R = Me, R1 = H, NO<sub>2</sub>, NH<sub>2</sub>; R = Ph, R1 = H) were obtained in 85-97% yield by treating acylaminobenzonitriles II with 5N HCl at room temperature II (R = CF<sub>3</sub>, R1 = H) did not cyclize under these conditions.

RX(2) OF 4            D    ==>   E



RX(2)            RCT   D 25116-00-1  
                  RGT   C 7647-01-0 HCl  
                  PRO   E 1769-24-0

RX(3) OF 4            F    ==>   G



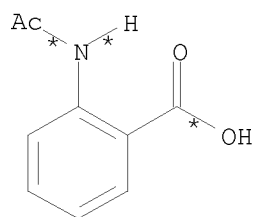
RX(3)            RCT   F 73894-39-0  
                  RGT   C 7647-01-0 HCl  
                  PRO   G 17329-24-7

RX(4) OF 4            H    ==>   I

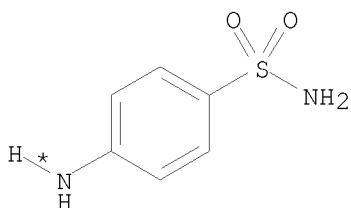




10/ 562,112

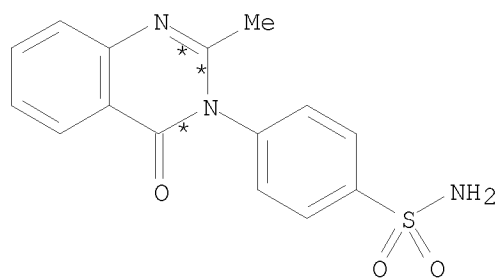


A



B

(1)  $\longrightarrow$

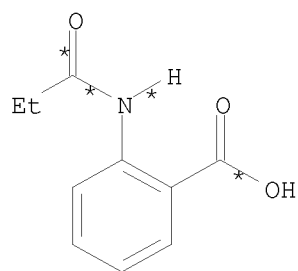


C

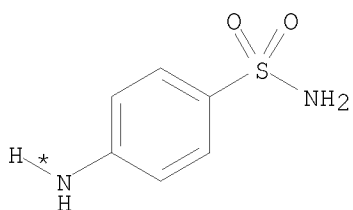
YIELD 80%

RX(1)      RCT    A 89-52-1, B 63-74-1  
             PRO    C 1232-38-8

RX(2) OF 26      D + B ==> E...



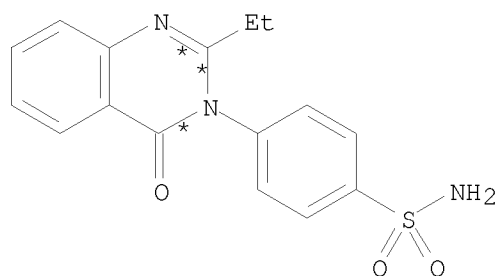
D



B

(2)  $\longrightarrow$

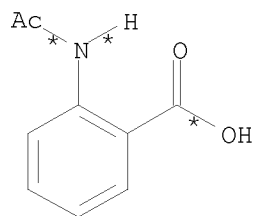
10/ 562,112



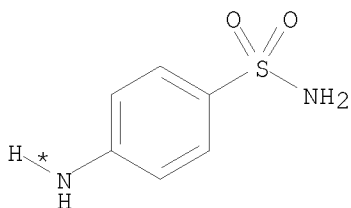
E  
YIELD 85%

RX(2) RCT D 19165-26-5, B 63-74-1  
PRO E 72723-65-0

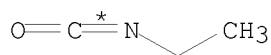
RX(14) OF 26 COMPOSED OF RX(1), RX(3)  
RX(14) A + B + F ==> G



A

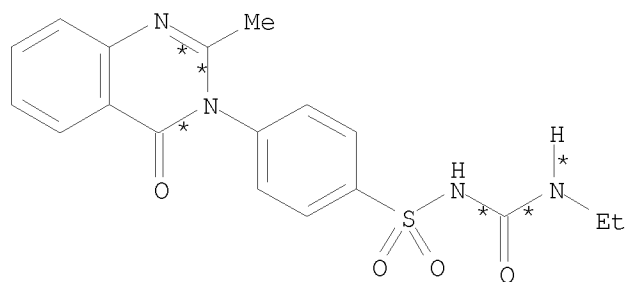


B



F

2  
STEPS  
→



G

RX(1) RCT A 89-52-1, B 63-74-1

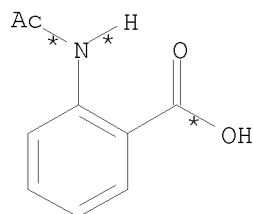
10/ 562,112

PRO C 1232-38-8

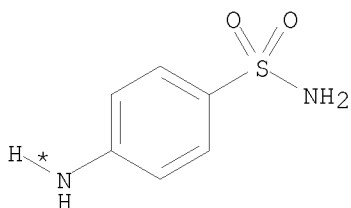
RX(3) RCT C 1232-38-8, F 109-90-0  
PRO G 72723-66-1  
CAT 584-08-7 K<sub>2</sub>CO<sub>3</sub>

RX(15) OF 26 COMPOSED OF RX(1), RX(4)

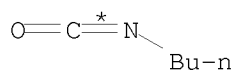
RX(15) A + B + I ==> J



A

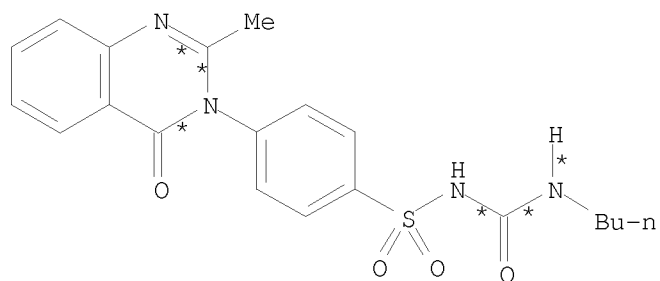


B



I

2  
STEPS  
→



J

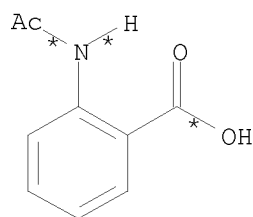
RX(1) RCT A 89-52-1, B 63-74-1  
PRO C 1232-38-8

RX(4) RCT C 1232-38-8, I 111-36-4  
PRO J 72723-68-3  
CAT 584-08-7 K<sub>2</sub>CO<sub>3</sub>

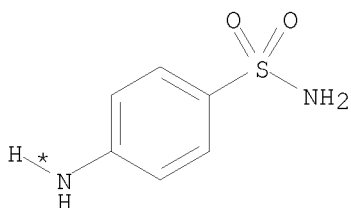
RX(16) OF 26 COMPOSED OF RX(1), RX(5)

RX(16) A + B + K ==> L

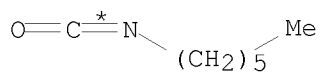
10/ 562,112



A

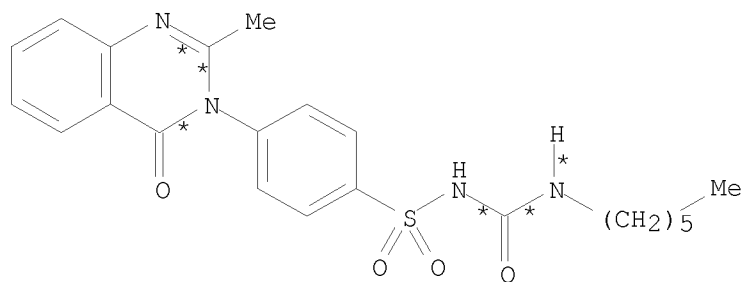


B



K

2  
STEPS  
→

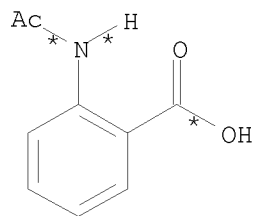


L

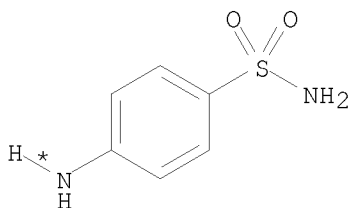
RX(1) RCT A 89-52-1, B 63-74-1  
PRO C 1232-38-8

RX(5) RCT C 1232-38-8, K 2525-62-4  
PRO L 343796-14-5  
CAT 584-08-7 K2CO3

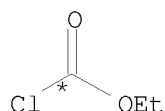
RX(17) OF 26 COMPOSED OF RX(1), RX(9)  
RX(17) A + B + Q ==> R



A



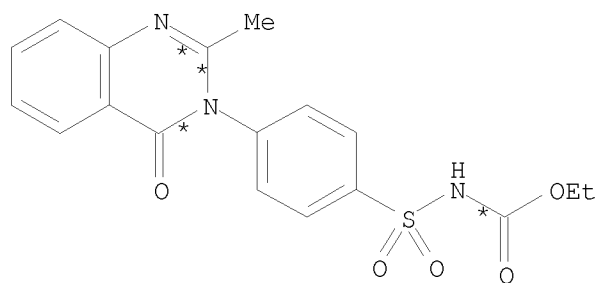
B



Q

2  
STEPS  
→

10/ 562,112



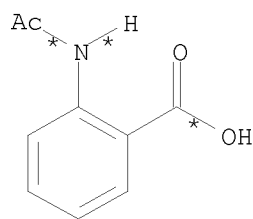
R

RX(1) RCT A 89-52-1, B 63-74-1  
PRO C 1232-38-8

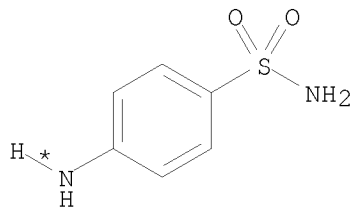
RX(9) RCT C 1232-38-8, Q 541-41-3  
PRO R 72723-76-3  
CAT 584-08-7 K<sub>2</sub>CO<sub>3</sub>

RX(18) OF 26 COMPOSED OF RX(1), RX(12)

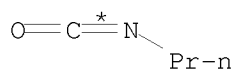
RX(18) A + B + N ==> W



A

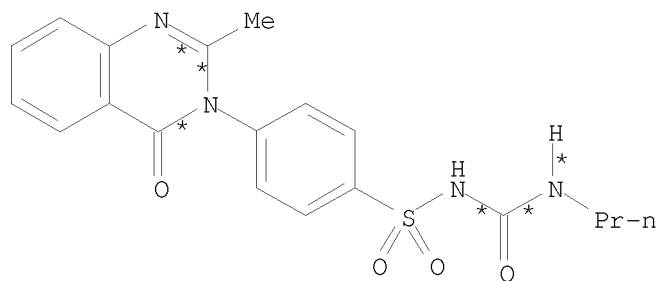


B



N

2  
STEPS  
→



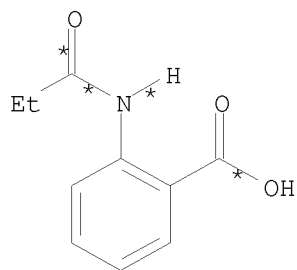
W

10/ 562,112

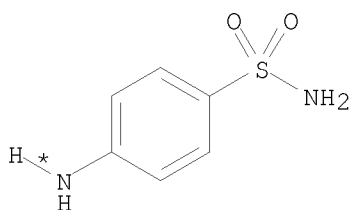
RX(1) RCT A 89-52-1, B 63-74-1  
PRO C 1232-38-8

RX(12) RCT C 1232-38-8, N 110-78-1  
PRO W 72723-67-2  
CAT 584-08-7 K2CO3

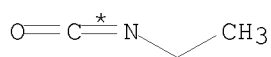
RX(19) OF 26 COMPOSED OF RX(2), RX(6)  
RX(19) D + B + F ==> M



D

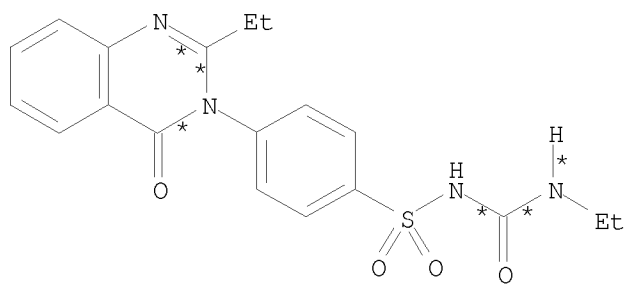


B



F

2  
STEPS  
→



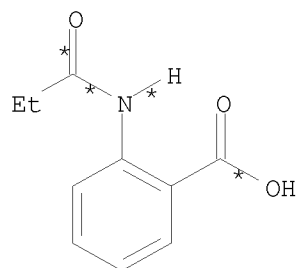
M

RX(2) RCT D 19165-26-5, B 63-74-1  
PRO E 72723-65-0

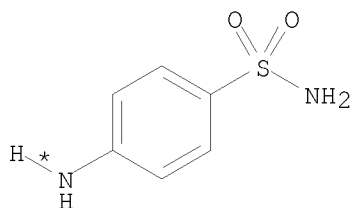
RX(6) RCT E 72723-65-0, F 109-90-0  
PRO M 72723-72-9  
CAT 584-08-7 K2CO3

RX(20) OF 26 COMPOSED OF RX(2), RX(7)  
RX(20) D + B + N ==> O

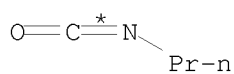
10/ 562,112



D

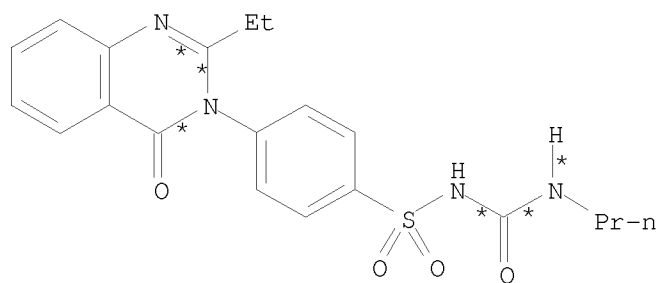


B



N

2  
STEPS  
→



O

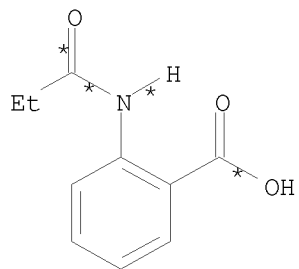
RX(2) RCT D 19165-26-5, B 63-74-1  
PRO E 72723-65-0

RX(7) RCT E 72723-65-0, N 110-78-1  
PRO O 72723-73-0  
CAT 584-08-7 K2CO3

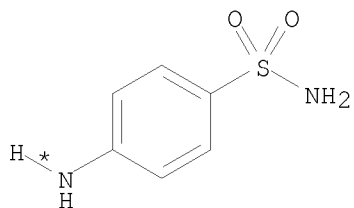
RX(21) OF 26 COMPOSED OF RX(2), RX(8)  
RX(21) D + B + I ==> P



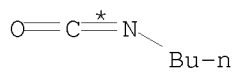
10/ 562,112



D

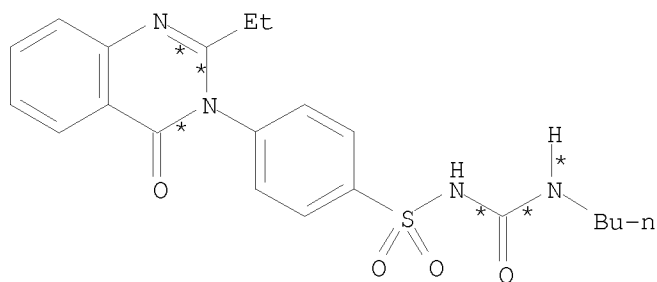


B



I

2  
STEPS  
→



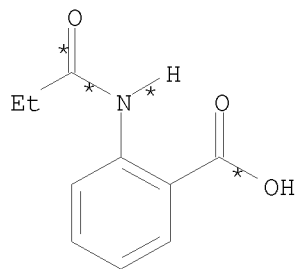
P

RX(2) RCT D 19165-26-5, B 63-74-1  
PRO E 72723-65-0

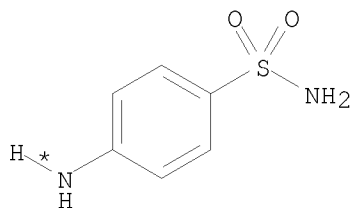
RX(8) RCT E 72723-65-0, I 111-36-4  
PRO P 72723-74-1  
CAT 584-08-7 K<sub>2</sub>CO<sub>3</sub>

RX(22) OF 26 COMPOSED OF RX(2), RX(13)  
RX(22) D + B + K ==> X

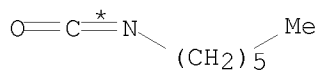
10/ 562,112



D

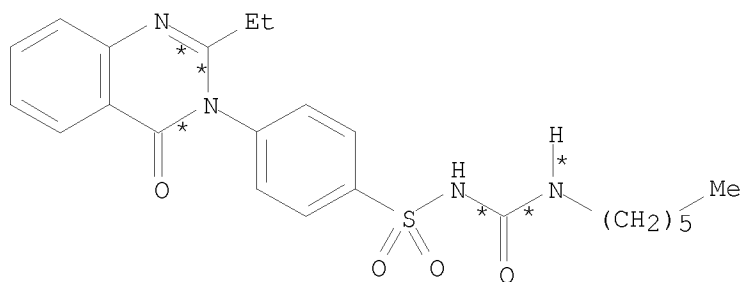


B



K

2  
STEPS  
→

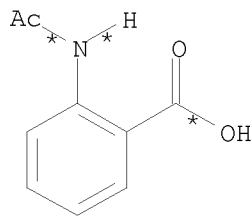


X

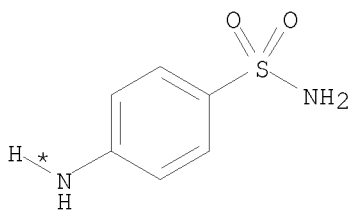
RX(2) RCT D 19165-26-5, B 63-74-1  
PRO E 72723-65-0

RX(13) RCT E 72723-65-0, K 2525-62-4  
PRO X 343796-84-9  
CAT 584-08-7 K2CO3

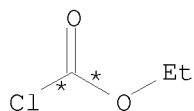
RX(25) OF 26 COMPOSED OF RX(1), RX(9), RX(10)  
RX(25) A + B + Q + S ==> T



A

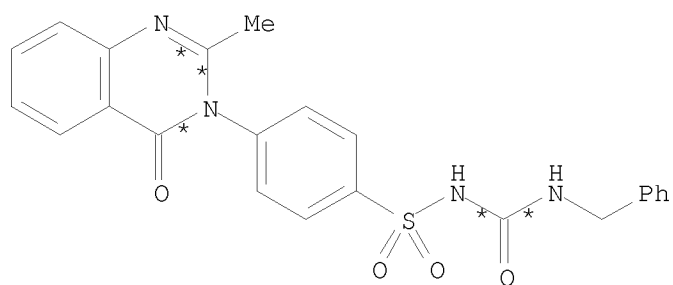
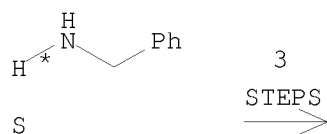


B



Q

10/ 562,112



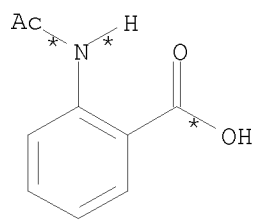
T  
YIELD 72%

RX(1)      RCT    A 89-52-1, B 63-74-1  
              PRO    C 1232-38-8

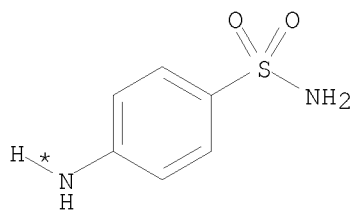
RX(9)      RCT    C 1232-38-8, Q 541-41-3  
              PRO    R 72723-76-3  
              CAT    584-08-7 K<sub>2</sub>CO<sub>3</sub>

RX(10)     RCT    R 72723-76-3, S 100-46-9  
              PRO    T 72723-70-7

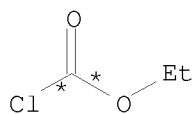
RX(26) OF 26 COMPOSED OF RX(1), RX(9), RX(11)  
 RX(26)      A + B + Q + U ==> V



A

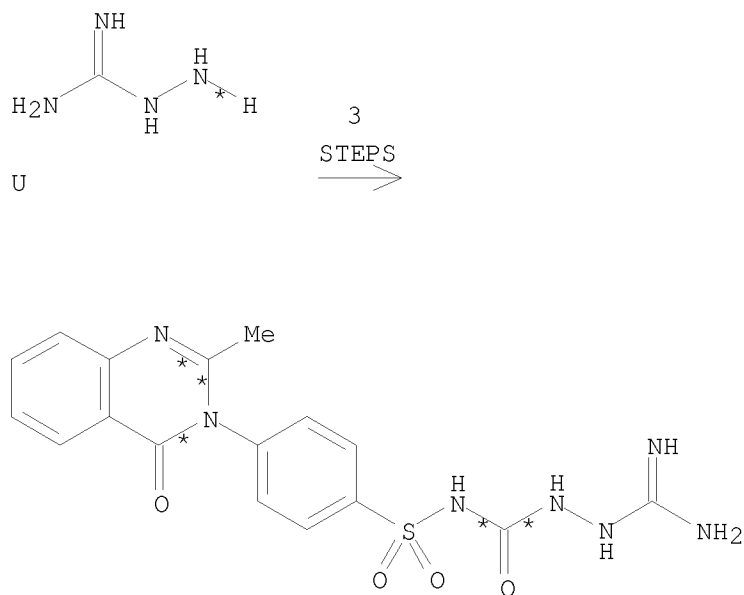


B



Q

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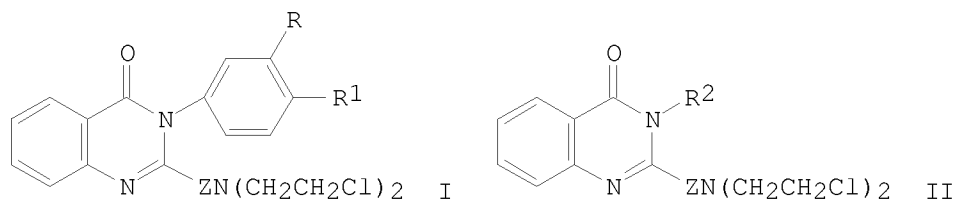
V  
YIELD 77%

RX(1) RCT A 89-52-1, B 63-74-1  
PRO C 1232-38-8

RX(9) RCT C 1232-38-8, Q 541-41-3  
PRO R 72723-76-3  
CAT 584-08-7 K2CO3

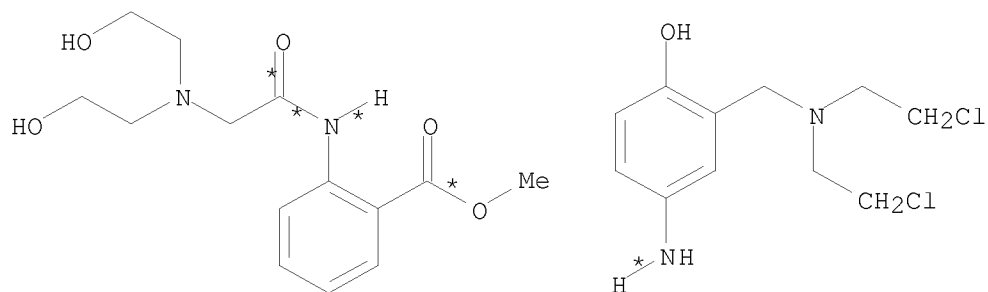
RX(11) RCT R 72723-76-3, U 79-17-4  
PRO V 72723-71-8

L3 ANSWER 233 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 92:58712 CASREACT  
TITLE: Study in nitrogen mustards, Part III. Synthesis of  
some 2-alkyl-3-aryl-4 (3H)-quinazolinone derivatives  
with nitrogen mustard moiety as possible antitumor  
agents  
AUTHOR(S): Singh, Pritpal; Gupta, I. S.  
CORPORATE SOURCE: Dep. Chem. Eng. Technol., Panjab Univ., Chandigarh,  
160 014, India  
SOURCE: Journal of the Indian Chemical Society (1979), 56(1),  
77-80  
CODEN: JICSAH; ISSN: 0019-4522  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Title quinazolinones I [ $Z = (CH_2)_n$  ( $n = 0-2$ ), CHMe;  $R = \text{e.g.}$   $CH_2N(CH_2CH_2OH)_2$ ,  $CH_2NHCH_2CH_2Br$ ;  $R_1 = OH, OMe, OEt$ ] (32 compds.) and II [ $Z = (CH_2)_n$  ( $n = 1, 2$ ), CHMe;  $R_2 = CH_2CH_2N(CH_2CH_2X)_2$  ( $X = Br, Cl, OH$ ),  $SO_2C_6H_4N(CH_2CH_2Cl)_2$ ] (10 compds.) were prepared from N-acyl anthranilates by condensing with anilines or hydrazides, resp. I and II contain mono or bifunctional nitrogen mustard groups attached to the quinazoline through an enzymatically-hydrolyzable linkage; they showed relatively low toxicity.

RX(4) OF 12            ...G + H ==> I...

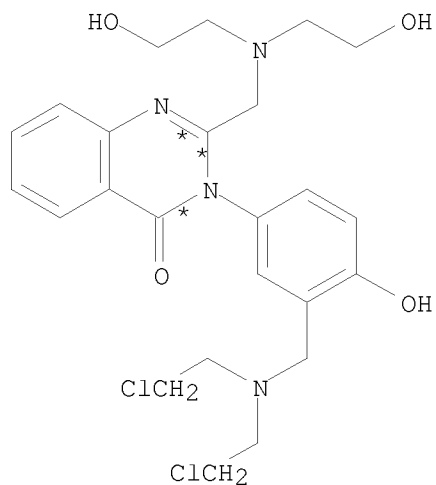


G

H

(4)  $\longrightarrow$

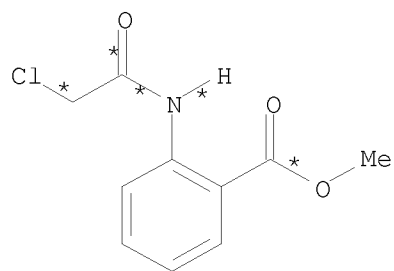
10/ 562,112



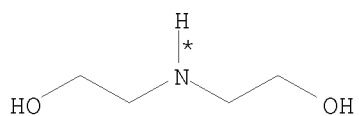
I  
YIELD 60%

RX(4) RCT G 72544-39-9, H 56538-41-1  
PRO I 72544-40-2

RX(8) OF 12 COMPOSED OF RX(3), RX(4)  
RX(8) E + F + H ==> I

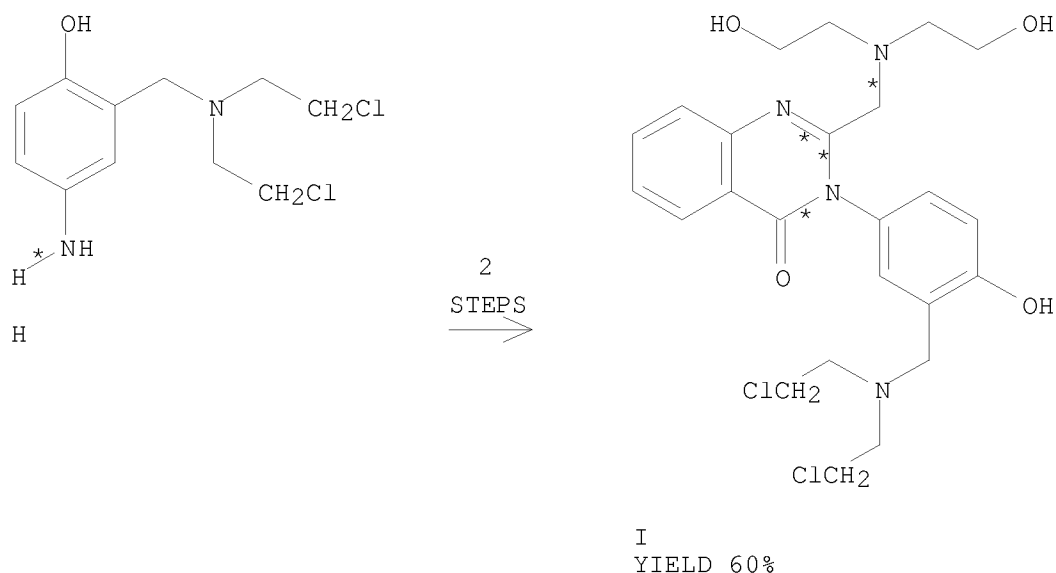


E



F

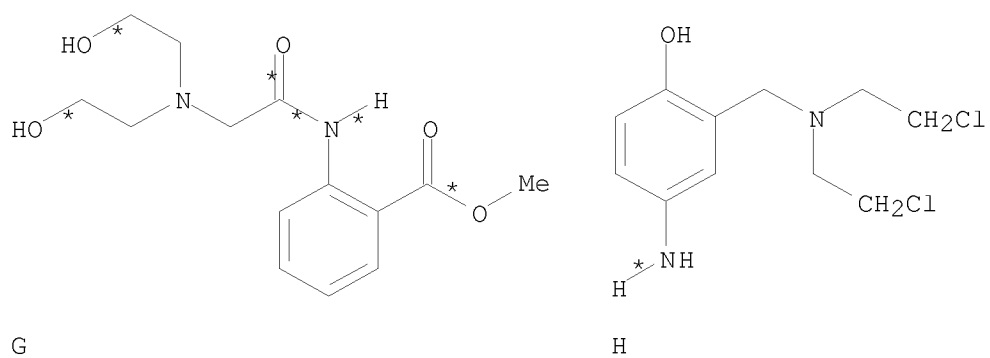
10/ 562,112



RX(3) RCT E 58915-18-7, F 111-42-2  
PRO G 72544-39-9

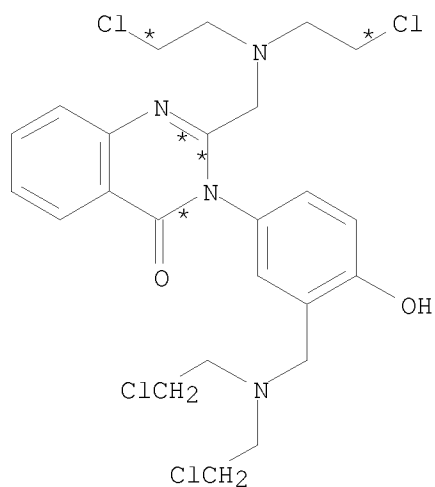
RX(4) RCT G 72544-39-9, H 56538-41-1  
PRO I 72544-40-2

RX(9) OF 12 COMPOSED OF RX(4), RX(5)  
RX(9) G + H ==> J



2  
STEPS  
→

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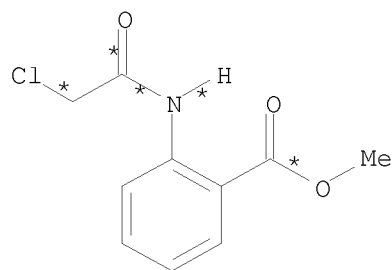


J  
YIELD 57%

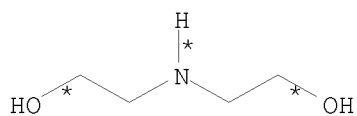
RX(4) RCT G 72544-39-9, H 56538-41-1  
PRO I 72544-40-2

RX(5) RCT I 72544-40-2  
RGT K 7719-09-7 SOCl2  
PRO J 72544-41-3

RX(11) OF 12 COMPOSED OF RX(3), RX(4), RX(5)  
RX(11) E + F + H ==> J

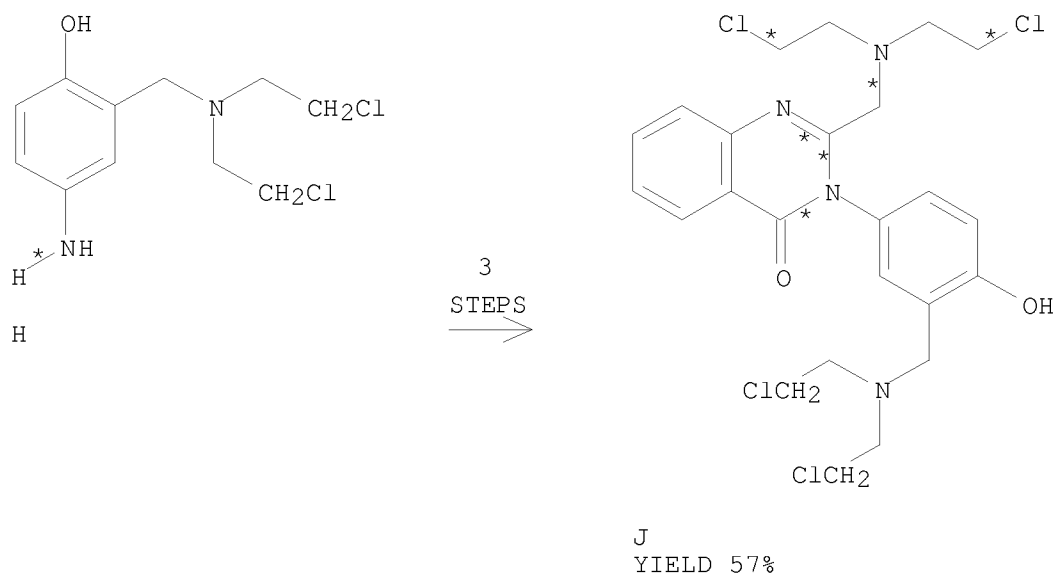


E



F



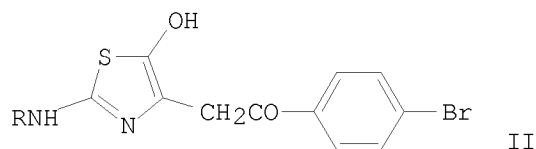


RX(3) RCT E 58915-18-7, F 111-42-2  
PRO G 72544-39-9

RX(4) RCT G 72544-39-9, H 56538-41-1  
PRO I 72544-40-2

RX(5) RCT I 72544-40-2  
RGT K 7719-09-7 SOC12  
PRO J 72544-41-3

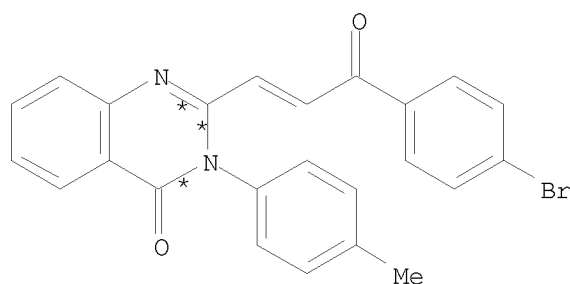
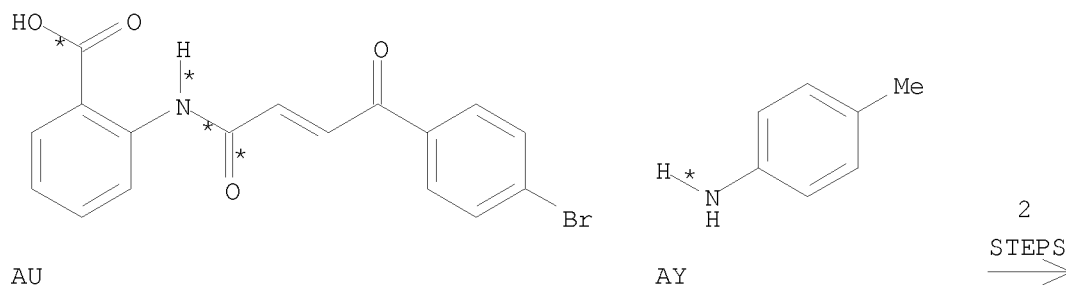
L3 ANSWER 234 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 92:41868 CASREACT  
TITLE: Some reactions with  $\beta$ -(p-bromobenzoyl)acrylic acid  
AUTHOR(S): Sammour, A.; Abdallah, M. M.; Essawy, A.; Elmobayed, M.  
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt  
SOURCE: Egyptian Journal of Chemistry (1979), Volume Date 1976, 19(6), 911-26  
CODEN: EGJCA3; ISSN: 0367-0422  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB 4-BrC<sub>6</sub>H<sub>4</sub>COCH:CHCO<sub>2</sub>H (I) reacted with piperidine to give  $\alpha$ -(4-bromophenacyl)-1-piperidineacetic acid; reaction of I with thioureas gave thiazoles II (R = H, CH<sub>2</sub>Ph, Ph), which were cyclized with N<sub>2</sub>H<sub>4</sub> or NH<sub>2</sub>OH to give thiazolopyridazines and thiazolooxazines resp. Friedel-Crafts alkylation of R<sub>1</sub>Ph (R<sub>1</sub> = H, Me, Et, CHMe<sub>2</sub>) with I gave 4-BrC<sub>6</sub>H<sub>4</sub>COCH<sub>2</sub>CH(CO<sub>2</sub>H)C<sub>6</sub>H<sub>4</sub>R-4 which, were cyclized to diarylfuranones with Ac<sub>2</sub>O or were condensed to pyridazinones with hydrazines or oxazinones with NH<sub>2</sub>OH. Michael reactions of I gave 4-BrC<sub>6</sub>H<sub>4</sub>COCH<sub>2</sub>CHR<sub>2</sub>CO<sub>2</sub>H [R<sub>2</sub> = CH(CO<sub>2</sub>Et)<sub>2</sub>, CH(CO<sub>2</sub>Me)CH<sub>2</sub>CO<sub>2</sub>Me], which were hydrolyzed and decarboxylated to 4-BrC<sub>6</sub>H<sub>4</sub>COCH<sub>2</sub>CH(CO<sub>2</sub>H)CHR<sub>3</sub>CO<sub>2</sub>H (R<sub>3</sub> = H, Me), which were cyclized to pyranones with Ac<sub>2</sub>O. 4-BrC<sub>6</sub>H<sub>4</sub>COCH:CHCOCl (III) reacted with 2-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H to give 2-HO<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>NHCOCH:CHCO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Br-4, which was cyclized to the benzoxazinone with Ac<sub>2</sub>O. The benzoxazinone was cleaved by arylamines; III was also used to acylate sulfa drugs.

RX(55) OF 57 COMPOSED OF RX(29), RX(31)

RX(55) AU + AY ==> AZ



YIELD 85%

RX(29) RCT AU 71553-50-9

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PRO AV 71553-51-0  
CAT 108-24-7 Ac2O

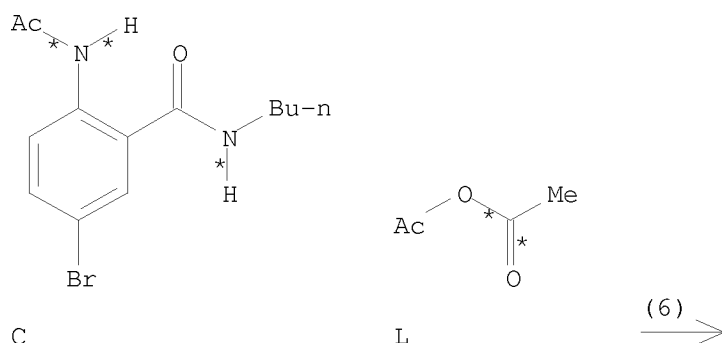
RX(31) RCT AV 71553-51-0, AY 106-49-0  
PRO AZ 71553-53-2

L3 ANSWER 235 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 91:211360 CASREACT  
TITLE: Some reactions with  
6-bromo-2-methyl-4H-3,1-benzoxazin-4-one and  
6-bromo-3-phenyl-2-methyl-4 (3H) -quinazolinone  
AUTHOR(S): Sammour, A.; Rabie, A.; Elhashash, M.; Sayed, M.  
CORPORATE SOURCE: Fac. Sci., Univ. Ain Shams, Cairo, Egypt  
SOURCE: Egyptian Journal of Chemistry (1978), Volume Date  
1976, 19(4), 571-88  
CODEN: EGJCA3; ISSN: 0367-0422  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

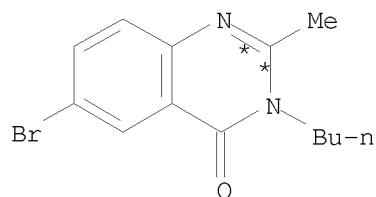
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Aminolysis of I with RNH<sub>2</sub> (R = alkyl, aryl) gave the acetanilides II and quinazolinones III via cyclocondensation. Condensation of I with aromatic aldehydes, ketones, and anhydrides, or phthalimide gave 2-styrylbenzoxazinones (IV; R<sub>1</sub> = aryl), bisbromobenzoxazinones (V; R<sub>2</sub> = Me, Ph; R<sub>3</sub> = Me, Ph, PhCH<sub>2</sub>), 1,3-diones (VI; R<sub>4</sub> = R<sub>5</sub> = H, R<sub>4</sub>R<sub>5</sub> = benzo), and the benzopyrrolidone derivative VII, resp. Condensation of VI (R<sub>4</sub>R<sub>5</sub> = benzo) with PhNH<sub>2</sub> and PhCH<sub>2</sub>CO<sub>2</sub>H gave VIII (Z = Z<sub>1</sub> = Z<sub>2</sub> = NPh and Z = Z<sub>1</sub> = O, Z<sub>2</sub> = CHPh, resp.). Condensation of I with hydrazines gave II (R = NH, arylamino), which was cyclized to III (R = NH<sub>2</sub>, arylamino) by Ac<sub>2</sub>O. Reaction of II (R = NH<sub>2</sub>) with PhCHO gave III (R = PhCH:N) and with MeCOCO<sub>2</sub>Et gave II (R = NHCOCH<sub>2</sub>COMe), which was cyclized to III (R = NHCOCH<sub>2</sub>COMe) by Ac<sub>2</sub>O.

RX(6) OF 85 ...C + L ==> M



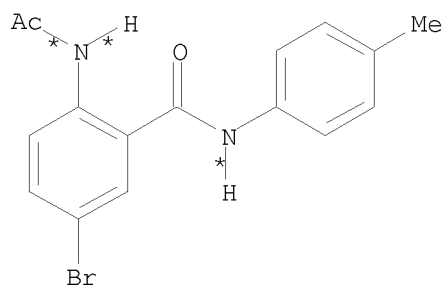
10/ 562,112



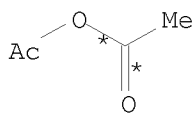
M  
YIELD 78%

RX(6) RCT C 71822-55-4, L 108-24-7  
PRO M 71822-61-2

RX(7) OF 85 ...E + L ==> N

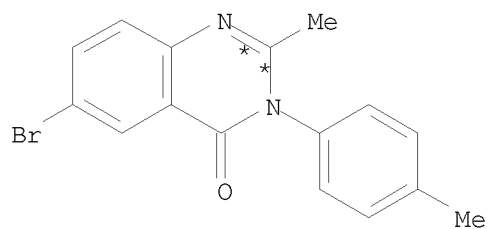


E



L

(7) >

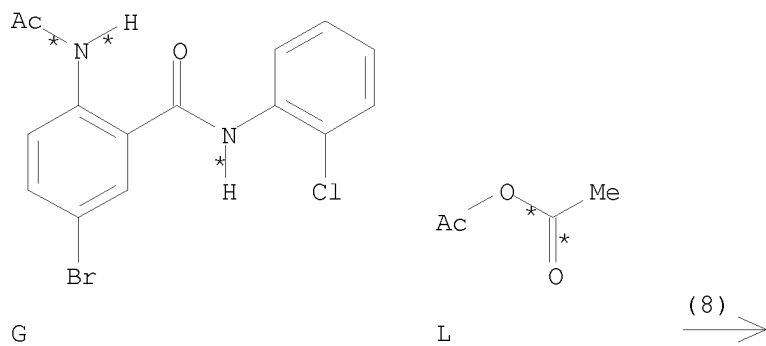


N  
YIELD 79%

RX(7) RCT E 71822-56-5, L 108-24-7  
PRO N 71822-62-3

RX(8) OF 85 ...G + L ==> O

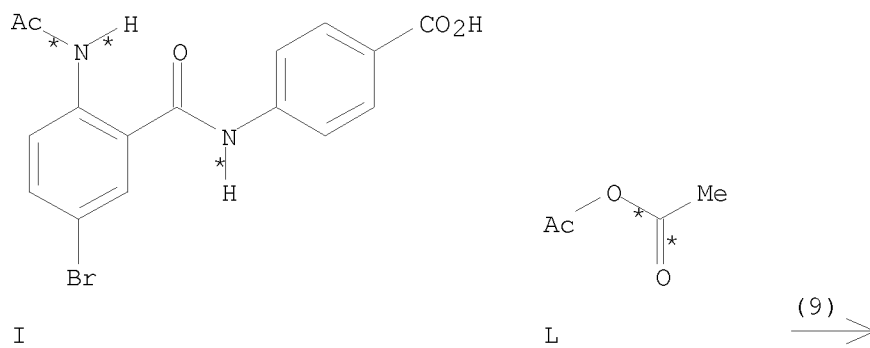
10/ 562,112



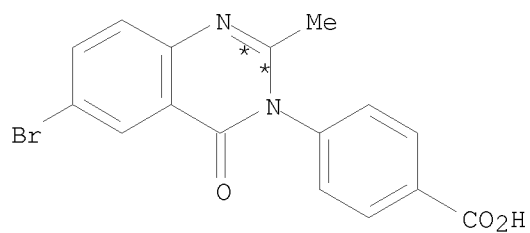
O  
YIELD 77%

RX(8) RCT G 71822-57-6, L 108-24-7  
 PRO O 19868-06-5

RX(9) OF 85 ...I + L ==> P



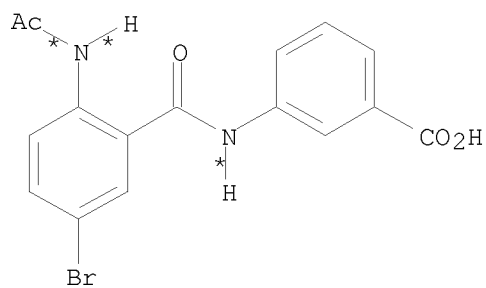
10/ 562,112



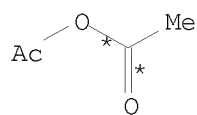
P  
YIELD 81%

RX(9) RCT I 71822-58-7, L 108-24-7  
PRO P 24295-50-9

RX(10) OF 85 ...K + L ==> Q

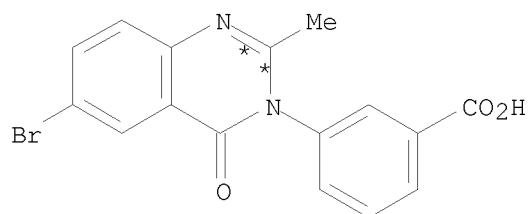


K



L

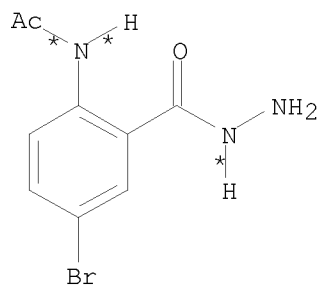
(10)  $\longrightarrow$



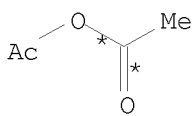
Q  
YIELD 79%

RX(10) RCT K 71822-59-8, L 108-24-7  
PRO Q 72005-21-1

RX(33) OF 85 ...BG + L ==> BH...

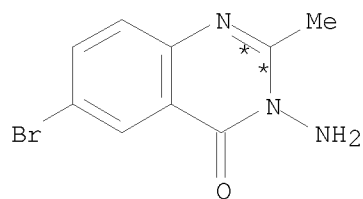


BG



L

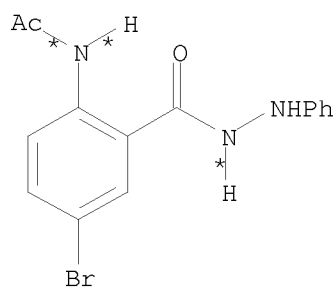
(33)



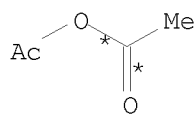
BH  
YIELD 70%

RX(33) RCT BG 71822-95-2, L 108-24-7  
PRO BH 71822-97-4

RX(34) OF 85 ...BD + L ==> BI



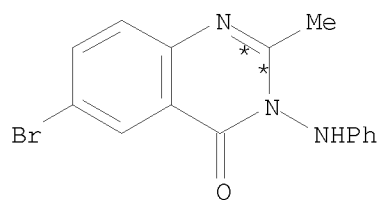
BD



L

(34)

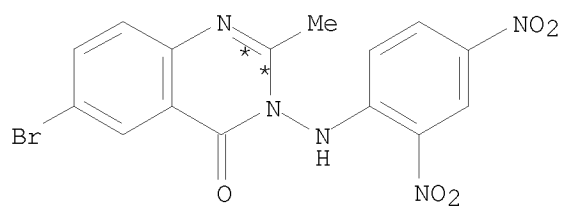
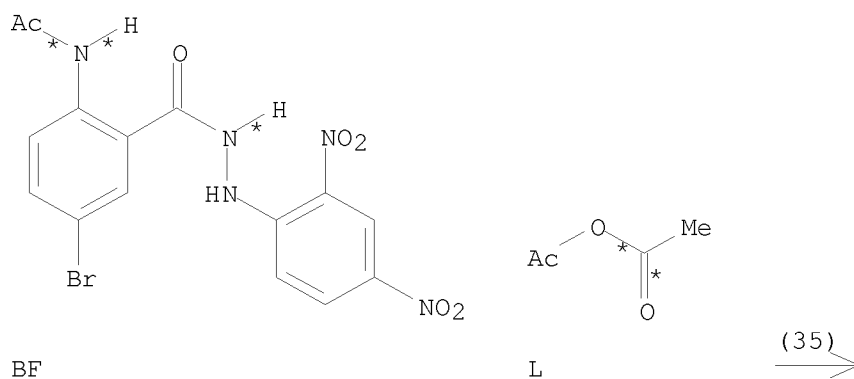
10/ 562,112



BI  
YIELD 81%

RX(34) RCT BD 71822-96-3, L 108-24-7  
PRO BI 71822-98-5

RX(35) OF 85 ...BF + L ==> BJ



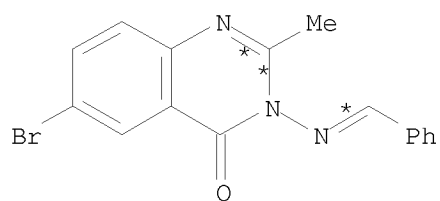
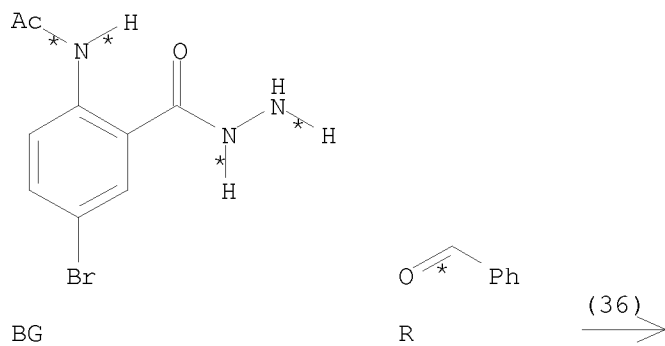
BJ  
YIELD 79%

RX(35) RCT BF 71861-26-2, L 108-24-7  
PRO BJ 71822-99-6

RX(36) OF 85 ...BG + R ==> BK



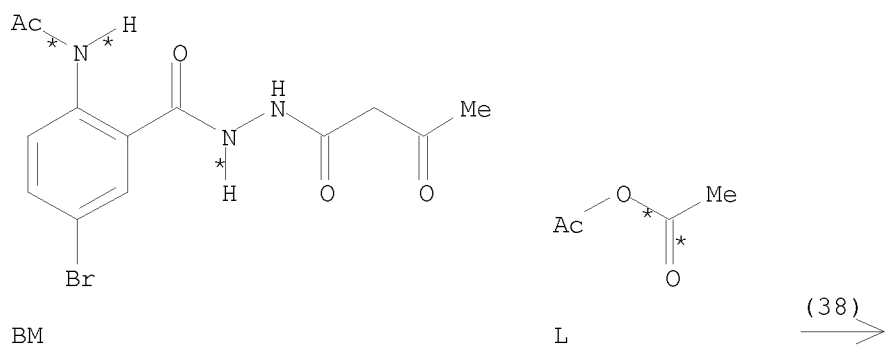
10/ 562,112



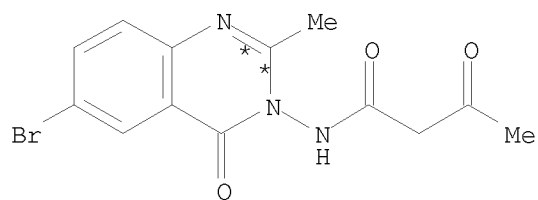
BK  
YIELD 71%

RX(36)      RCT    BG 71822-95-2, R 100-52-7  
              PRO    BK 71823-00-2

RX(38) OF 85      ...BM + L ==> BN



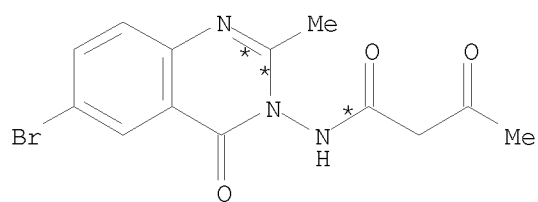
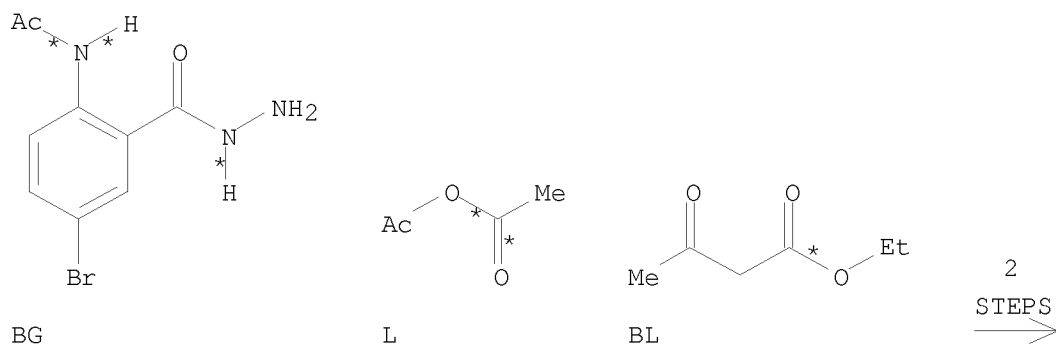
10/ 562,112



BN  
YIELD 68%

RX(38) RCT BM 71823-01-3, L 108-24-7  
PRO BN 71823-02-4

RX(57) OF 85 COMPOSED OF RX(33), RX(39)  
RX(57) BG + L + BL ==> BN

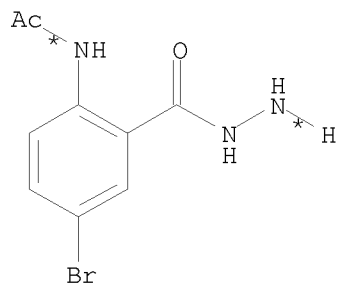


BN  
YIELD 65%

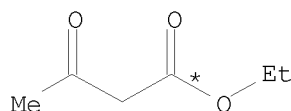
RX(33) RCT BG 71822-95-2, L 108-24-7  
PRO BH 71822-97-4

RX(39) RCT BH 71822-97-4, BL 141-97-9  
PRO BN 71823-02-4

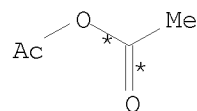
RX(58) OF 85 COMPOSED OF RX(37), RX(38)  
RX(58) BG + BL + L ==> BN



BG

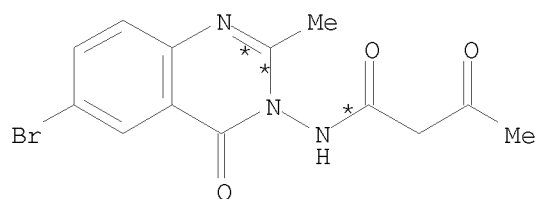


BL



L

2  
STEPS  
→

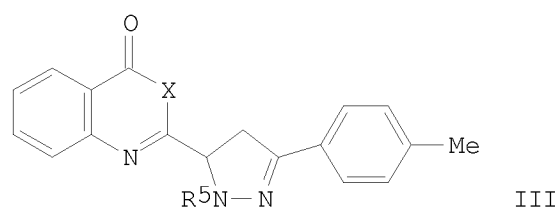
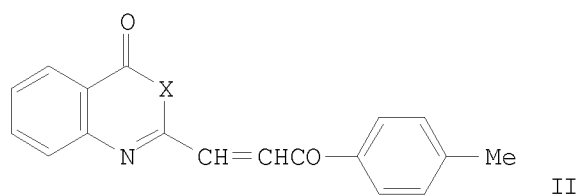


BN  
YIELD 68%

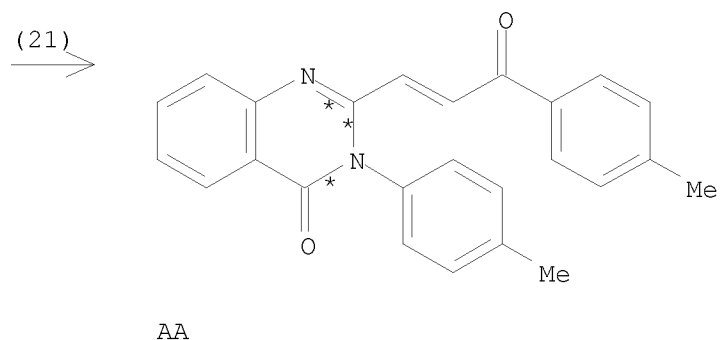
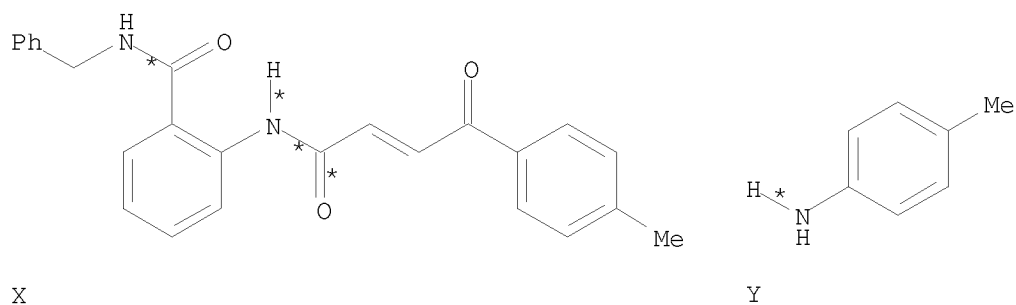
RX(37) RCT BG 71822-95-2, BL 141-97-9  
PRO BM 71823-01-3

RX(38) RCT BM 71823-01-3, L 108-24-7  
PRO BN 71823-02-4

L3 ANSWER 236 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 91:175295 CASREACT  
TITLE: Reactions with the amides and chlorides of some  
 $\beta$ -aroylacrylic acids  
AUTHOR(S): Sammour, A.; Afify, A. A.; Abdallah, M.; Soliman, E.  
A.  
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt  
SOURCE: Egyptian Journal of Chemistry (1979), Volume Date  
1976, 19(6), 1109-16  
CODEN: EGJCA3; ISSN: 0367-0422  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



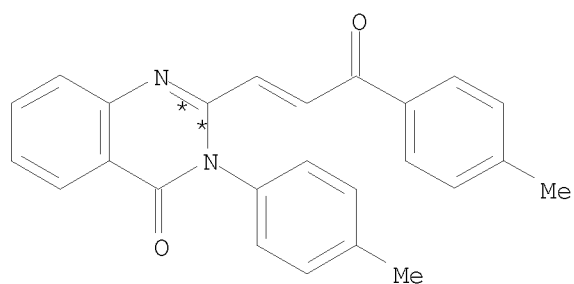
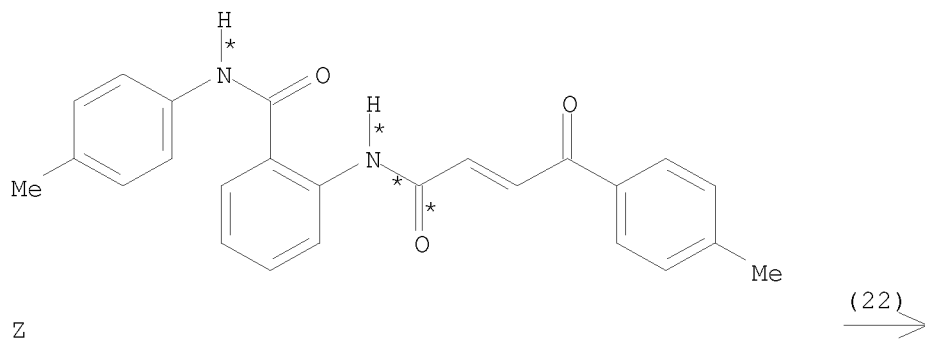
AB RCOCH:CHCONHCSNHR1 (R = 4-MeC6H4, 2-naphthyl; R1 = H, CH2Ph) were prepared by treating RCOCH:CHCONHC6H4R2-4 (R2 = H, Me, OMe) or 4-MeC6H4COCH:CHCOC1 (I) with H2NCSNHR1. 4-MeC6H4COCH:CHCONHC6H4SO2NHR3-4 [R3 = H, C(:NH)NH2, 4-methyl-2-pyrimidinyl] were obtained from I and H2NC6H4SO2NHR3-4. I reacted with 2-H2NC6H4CO2H to give 2-HO2CC6H4NHCOCCH:CHCOC6H4Me-4, which cyclized to the benzoxazinone II (X = O). Reaction of II (X = O) with amines R4NH2 in EtOH gave 2-R4NHCOC6H4NHCOCCH:CHCOC6H4Me-4 (R4 = CH2Ph, 4-MeC6H4), but reaction with 4-MeC6H4NH2 at 170° gave II (X = NC6H4Me-4). Reaction of II (X = O) with N2H4 gave III (X = O, NNH2, R5 = H), whereas with PhNHNH2 only III (X = NNHPh, R5 = Ph) was obtained.

$$\text{RX(21) OF 37} \quad \dots X + Y \implies \text{AA}$$


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RX(21) RCT X 71703-79-2, Y 106-49-0  
PRO AA 71703-81-6

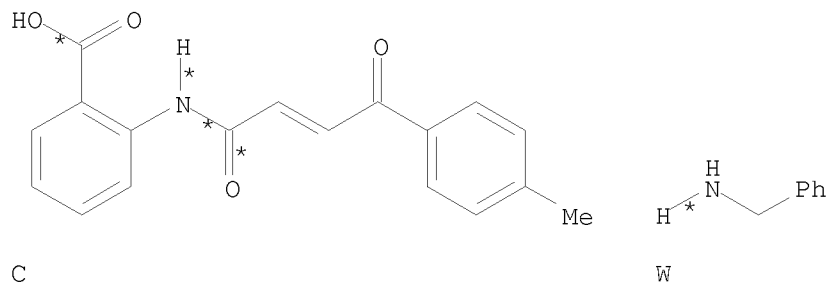
RX(22) OF 37 ...Z ==> AA



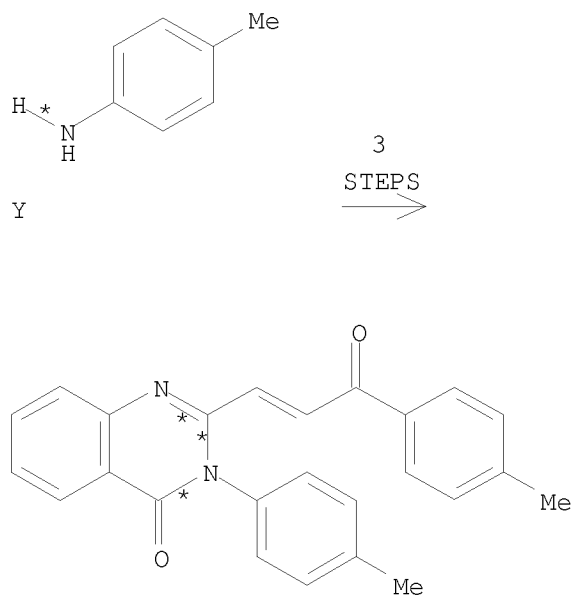
AA

RX(22) RCT Z 71703-80-5  
PRO AA 71703-81-6  
CAT 106-49-0 4-MeC6H4NH2

RX(34) OF 37 COMPOSED OF RX(18), RX(19), RX(21)  
RX(34) C + W + Y ==> AA



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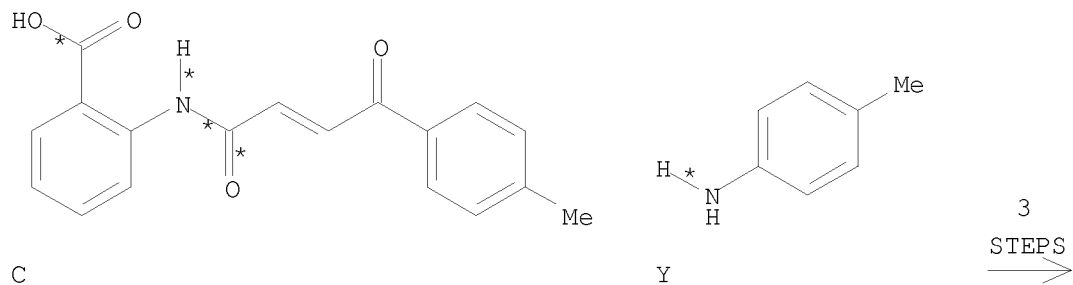


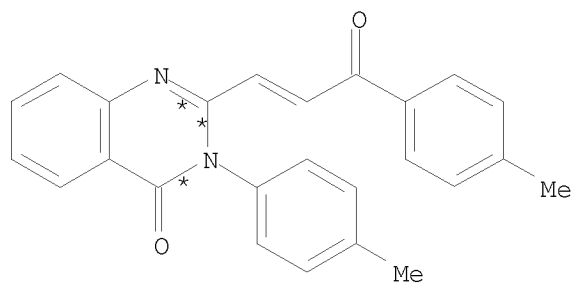
RX(18) RCT C 70596-64-4  
 PRO U 71703-78-1  
 CAT 108-24-7 Ac2O

RX(19) RCT U 71703-78-1, W 100-46-9  
 PRO X 71703-79-2

RX(21) RCT X 71703-79-2, Y 106-49-0  
 PRO AA 71703-81-6

RX(35) OF 37 COMPOSED OF RX(18), RX(20), RX(22)  
 RX(35) C + Y ==> AA

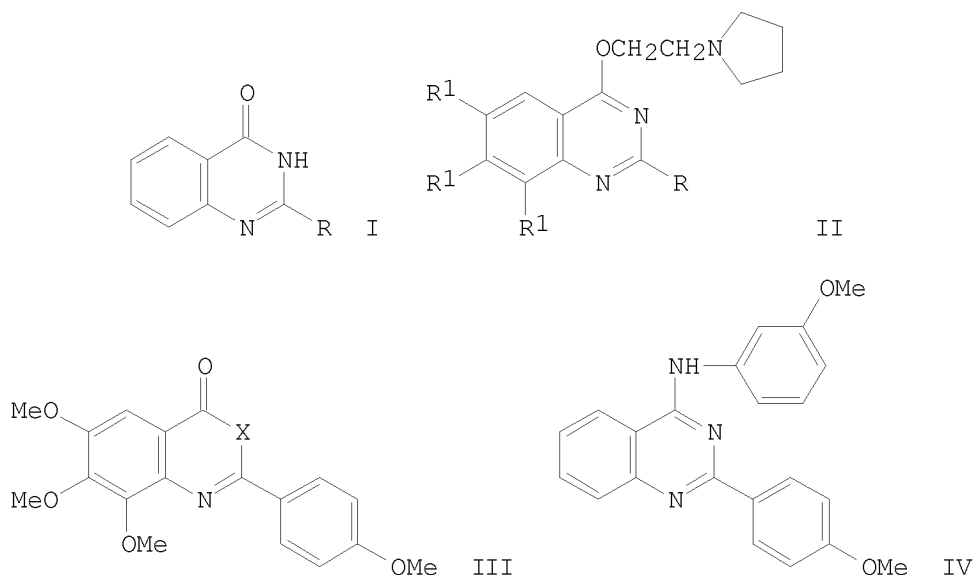




AA

RX(18) RCT C 70596-64-4  
 PRO U 71703-78-1  
 CAT 108-24-7 Ac2O  
  
 RX(20) RCT U 71703-78-1, Y 106-49-0  
 PRO Z 71703-80-5  
  
 RX(22) RCT Z 71703-80-5  
 PRO AA 71703-81-6  
 CAT 106-49-0 4-MeC6H4NH2

L3 ANSWER 237 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 91:157681 CASREACT  
 TITLE: Heterocyclic compounds. XII. Quinazoline derivatives  
 as potential antifertility agents  
 AUTHOR(S): Manhas, M. S.; Hoffman, W. A., III; Bose, A. K.  
 CORPORATE SOURCE: Dep. Chem. Chem. Eng., Stevens Inst. Technol.,  
 Hoboken, NJ, 07030, USA  
 SOURCE: Journal of Heterocyclic Chemistry (1979), 16(4),  
 711-15  
 CODEN: JHTCAD; ISSN: 0022-152X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

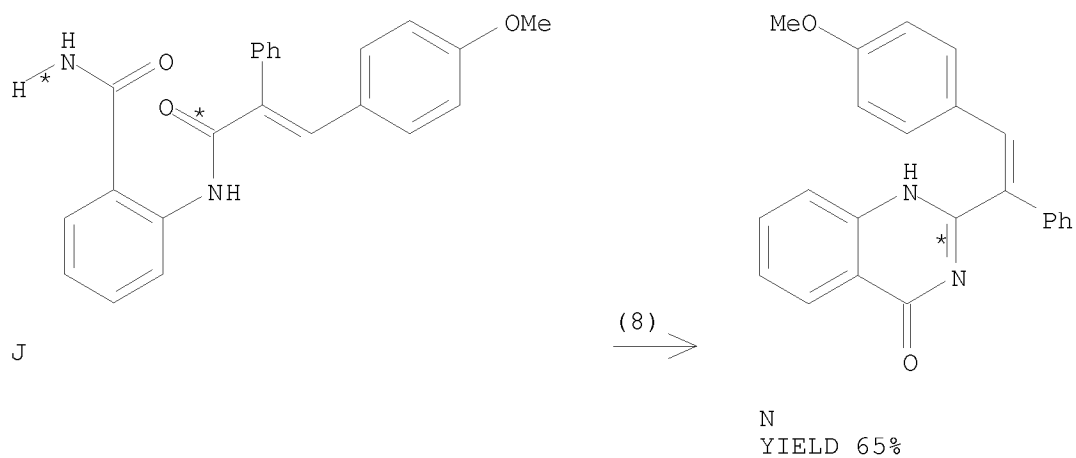


AB    Acylation of 2-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CONH<sub>2</sub> by RCOCl [R = 4-MeOC<sub>6</sub>H<sub>4</sub>, 4-MeOC<sub>6</sub>H<sub>4</sub>CH:CPh, α-benzylidene-3,4-dimethoxybenzyl, 3,4-methylenedioxyphenyl] gave 2-(RCONH)C<sub>6</sub>H<sub>4</sub>CONH<sub>2</sub>, which cyclized in refluxing Ph<sub>2</sub>O to give the corresponding quinazolinones I. Chlorination of I by POCl<sub>3</sub> followed by substitution reaction with 2-pyrrolidinoethanol Na salt gave ethoxyquinazolines II (R as defined above; R<sub>1</sub> = H). Hydrogenation of Me 3,4,5-trimethoxy-2-nitrobenzoate over Pt/C followed by acylation with 4-MeOC<sub>6</sub>H<sub>4</sub>COCl gave Me 2-(p-methoxybenzamido)-3,4,5-trimethoxybenzoate, which underwent cyclocondensation in refluxing C<sub>6</sub>H<sub>6</sub> containing NaOMe to give the benzoxazinone III (X = O). Treatment of III (X = O) with NH<sub>3</sub> in MeOH under pressure gave III (X = NH), which underwent chlorination and substitution reaction with pyrrolidinoethanol Na salt to give II (R = 4-MeOC<sub>6</sub>H<sub>4</sub>; R<sub>1</sub> = MeO). Reaction of I (R = 4-MeOC<sub>6</sub>H<sub>4</sub>) with P<sub>2</sub>S<sub>5</sub> gave the corresponding quinazolinethione, which underwent S-methylation with Me iodide and then substitution reaction with 3-MeOC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> to give the anilinoquinazoline IV. II (R = 4-MeOC<sub>6</sub>H<sub>4</sub>, α-benzylidene-3,4,5-trimethoxybenzyl, 3,4-methylenedioxyphenyl; R<sub>1</sub> = H) and IV possessed low level postcoital contraceptive activity in rats.

RX(8) OF 82      ...J ==> N...

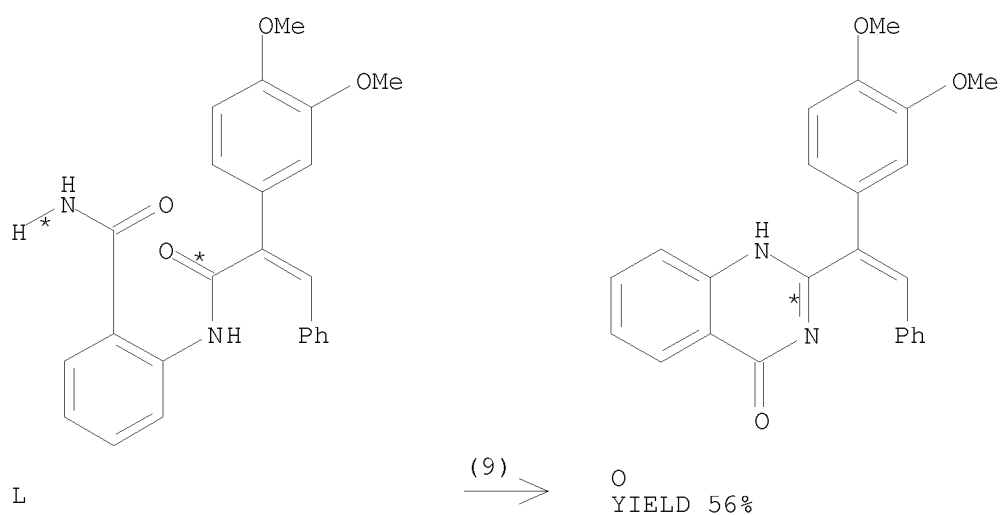


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RX(8) RCT J 71628-56-3  
PRO N 344878-36-0

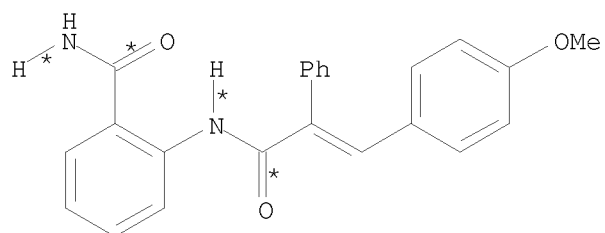
RX(9) OF 82 ...L  $\implies$  O...



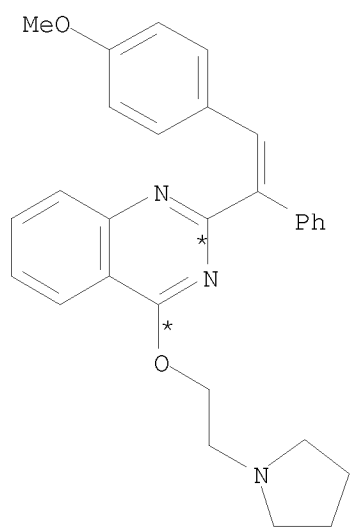
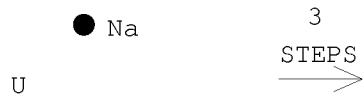
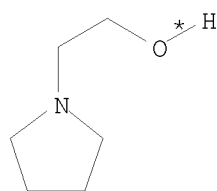
RX(9) RCT L 344878-90-6  
PRO O 344878-48-4

RX(66) OF 82 COMPOSED OF RX(8), RX(10), RX(14)  
RX(66) J + U  $\implies$  W

10/ 562,112



J



W

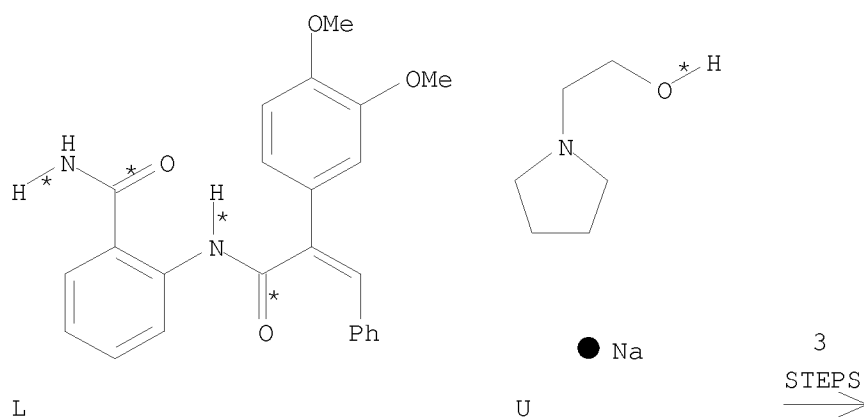
YIELD 37%

RX(8) RCT J 71628-56-3  
PRO N 344878-36-0

RX(10) RCT N 344878-36-0  
RGT Q 10025-87-3 POC13  
PRO P 344878-35-9

RX(14) RCT P 344878-35-9, U 71628-68-7  
PRO W 344909-05-3

RX(68) OF 82 COMPOSED OF RX(9), RX(11), RX(15)  
RX(68) L + U ==> X



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(9) RCT L 344878-90-6  
PRO O 344878-48-4

RX(11) RCT O 344878-48-4  
RGT Q 10025-87-3 POC13  
PRO R 344878-46-2

RX(15) RCT R 344878-46-2, U 71628-68-7  
PRO X 344909-41-7

L3 ANSWER 238 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 91:123700 CASREACT

TITLE: Studies in quinazolones: Part I. Synthesis and spectral characteristics of substituted 2-isopropyl-4(3H)-quinazolones

AUTHOR(S): Joshi, B. P.; Hosangadi, B. D.

CORPORATE SOURCE: Dep. Chem., Univ. Bombay, Bombay, 400098, India

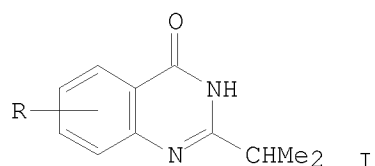
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1978), 16B(12), 1067-72

CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

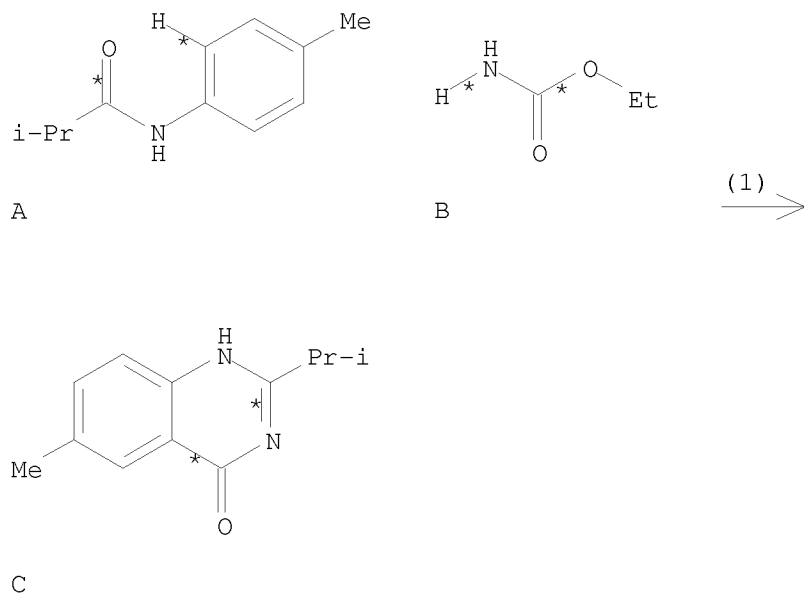
LANGUAGE: English

GI



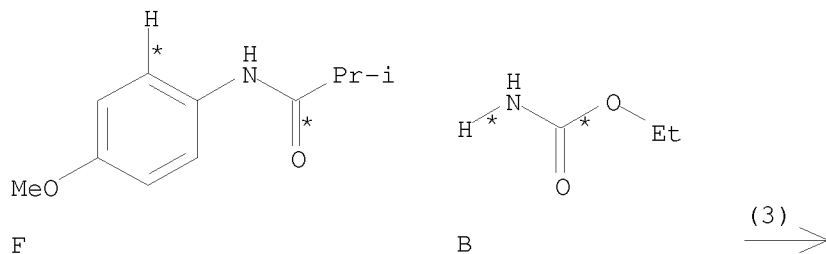
AB Approx. 10 2-isopropyl-4(3H)-quinazolones (I, R = Me, OMe, OEt, benzo) and their corresponding N-Me derivs. were synthesized by cyclization of EtO<sub>2</sub>CNH<sub>2</sub> with isobutyranilides, and their UV, IR and PMR spectral data discussed. Direct oxidation of 2-isopropyl-6-methyl-4(3H)-quinazolone with H<sub>2</sub>O<sub>2</sub>-AcOH gave 2-acetoxyisopropyl-6-methyl-4(3H)-quinazolone. This was the first acetoxylation of heterocyclic N-oxides in aqueous medium.

RX(1) OF 33 A + B ==> C...

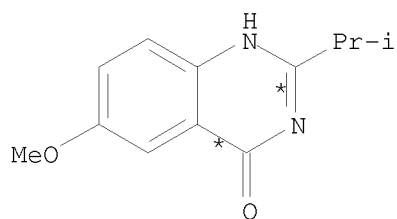


RX(1) RCT A 6876-49-9, B 51-79-6  
PRO C 71182-14-4

RX(3) OF 33 F + B ==> G...



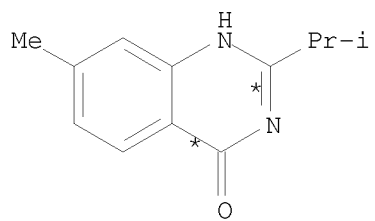
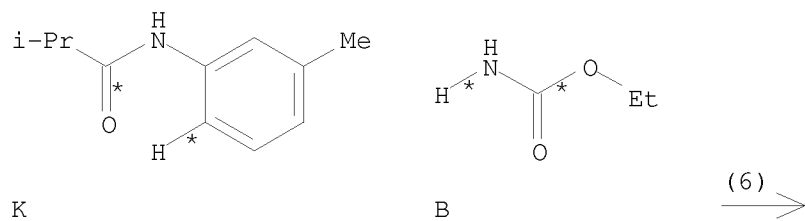
10/ 562,112



G

RX(3) RCT F 6642-37-1, B 51-79-6  
PRO G 71182-16-6

RX(6) OF 33 K + B ==> L...

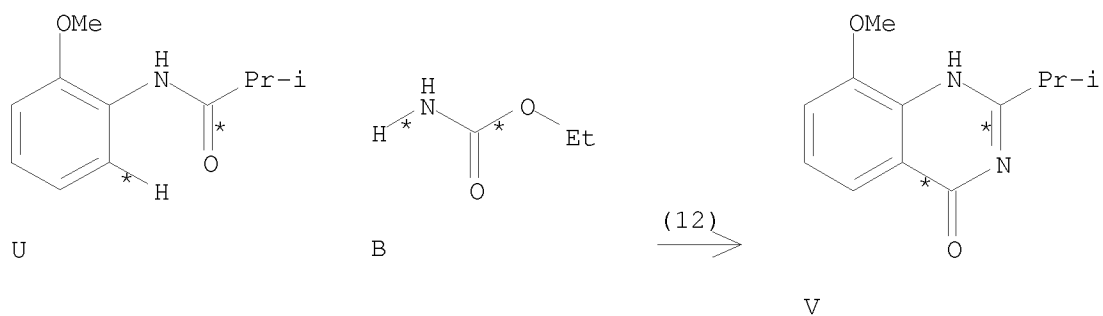


L

RX(6) RCT K 7146-00-1, B 51-79-6  
PRO L 71182-20-2

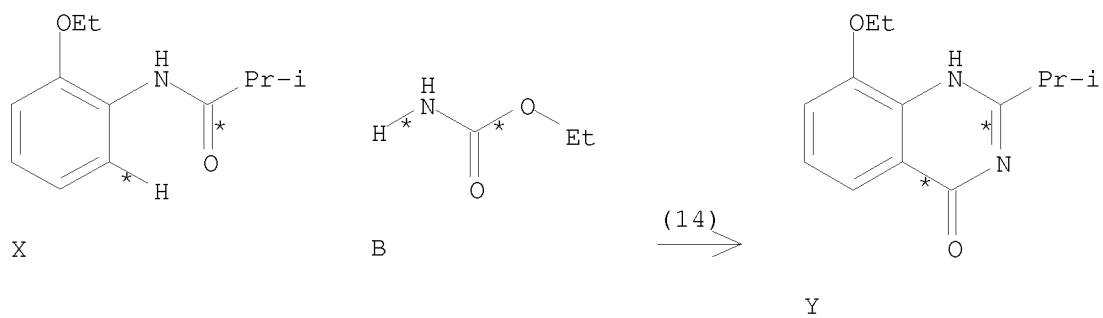
RX(12) OF 33 U + B ==> V...

10/ 562,112



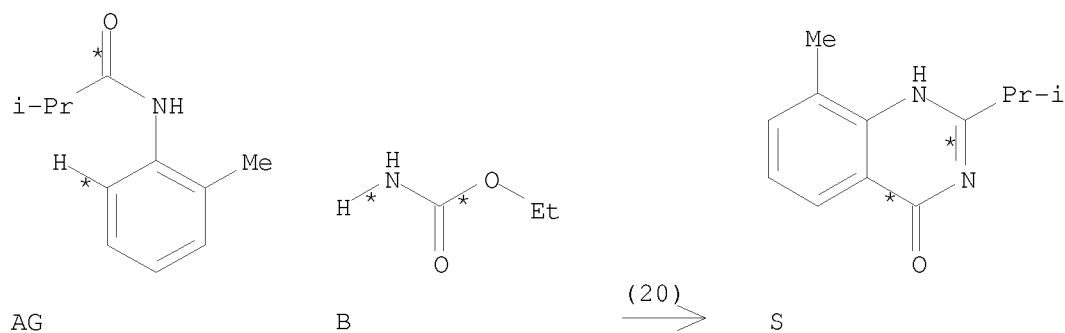
RX(12) RCT U 71182-38-2, B 51-79-6  
PRO V 71182-27-9

RX(14) OF 33 X + B  $\implies$  Y...



RX(14) RCT X 71182-39-3, B 51-79-6  
PRO Y 71182-29-1

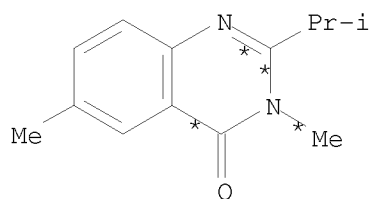
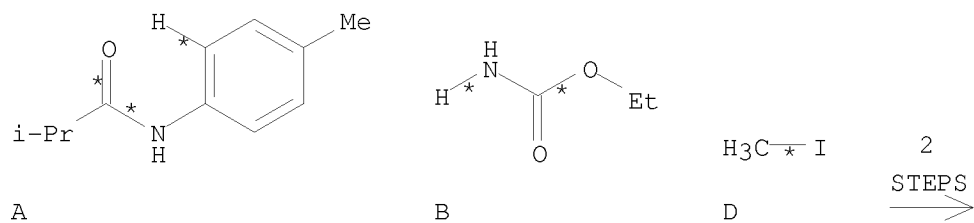
RX(20) OF 33 AG + B  $\implies$  S...



RX(20) RCT AG 55577-63-4, B 51-79-6  
PRO S 71381-27-6

10/ 562,112

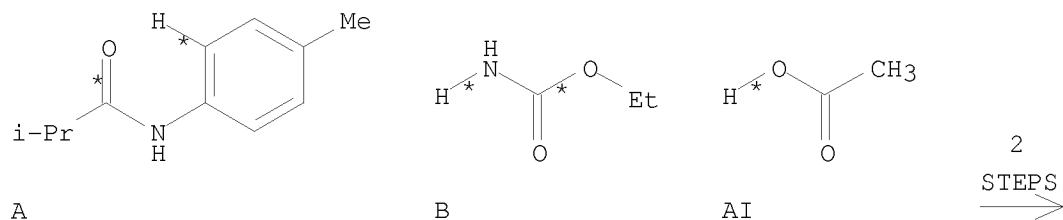
RX(23) OF 33 COMPOSED OF RX(1), RX(2)  
RX(23) A + B + D ==> E



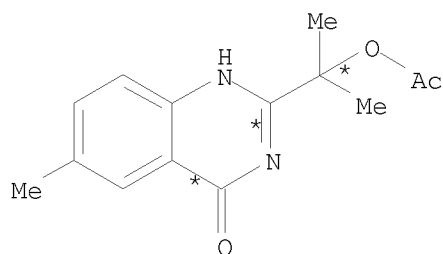
RX(1) RCT A 6876-49-9, B 51-79-6  
PRO C 71182-14-4

RX(2) RCT C 71182-14-4, D 74-88-4  
PRO E 71182-15-5

RX(24) OF 33 COMPOSED OF RX(1), RX(22)  
RX(24) A + B + AI ==> AJ



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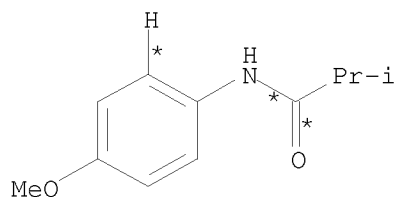


AJ

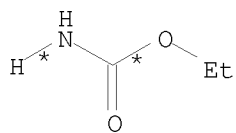
RX(1) RCT A 6876-49-9, B 51-79-6  
PRO C 71182-14-4

RX(22) RCT C 71182-14-4, AI 64-19-7  
RGT AK 7722-84-1 H2O2  
PRO AJ 71182-35-9

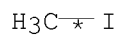
RX(25) OF 33 COMPOSED OF RX(3), RX(4)  
RX(25) F + B + D ==> H



F

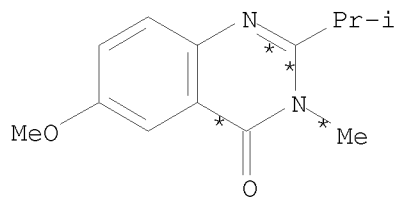


B



D

2  
STEPS  
→



H

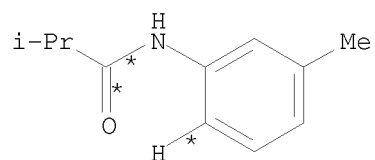
RX(3) RCT F 6642-37-1, B 51-79-6  
PRO G 71182-16-6

RX(4) RCT G 71182-16-6, D 74-88-4  
PRO H 71182-17-7

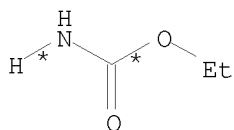
RX(26) OF 33 COMPOSED OF RX(6), RX(19)  
RX(26) K + B + D ==> AF



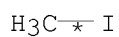
10/ 562,112



K

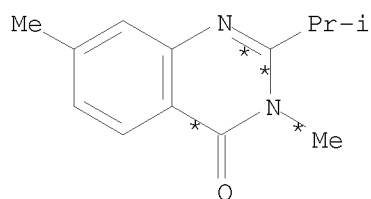


B



D

2  
STEPS  
→

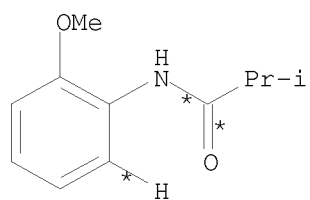


AF

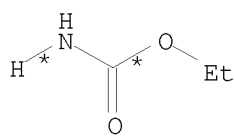
RX(6) RCT K 7146-00-1, B 51-79-6  
PRO L 71182-20-2

RX(19) RCT L 71182-20-2, D 74-88-4  
PRO AF 71182-21-3

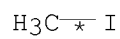
RX(29) OF 33 COMPOSED OF RX(12), RX(13)  
RX(29) U + B + D ==> W



U

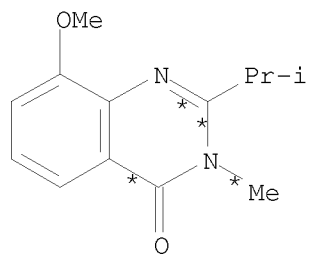


B



D

2  
STEPS  
→



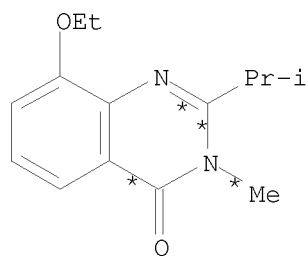
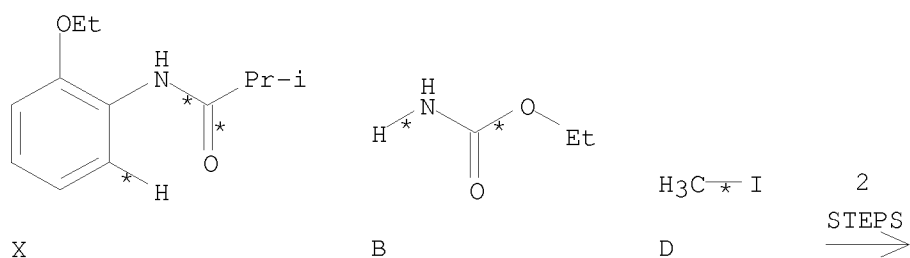
W

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RX(12) RCT U 71182-38-2, B 51-79-6  
PRO V 71182-27-9

RX(13) RCT V 71182-27-9, D 74-88-4  
PRO W 71182-28-0

RX(30) OF 33 COMPOSED OF RX(14), RX(15)  
RX(30) X + B + D ==> Z

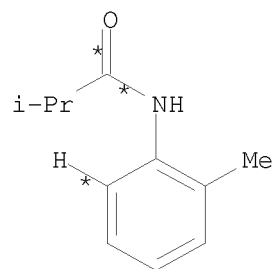


Z

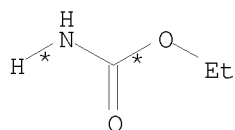
RX(14) RCT X 71182-39-3, B 51-79-6  
PRO Y 71182-29-1

RX(15) RCT Y 71182-29-1, D 74-88-4  
PRO Z 71182-30-4

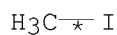
RX(32) OF 33 COMPOSED OF RX(20), RX(11)  
RX(32) AG + B + D ==> T



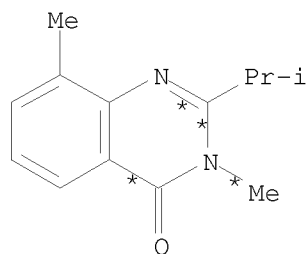
AG



B



D

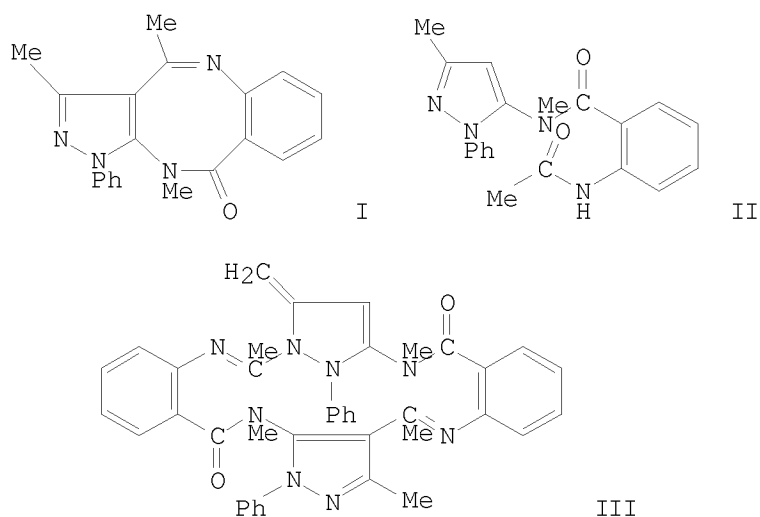


T

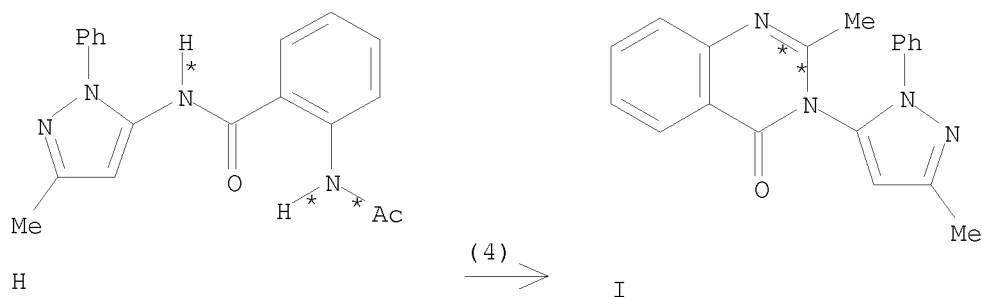
RX(20) RCT AG 55577-63-4, B 51-79-6  
 PRO S 71381-27-6

RX(11) RCT S 71381-27-6, D 74-88-4  
 PRO T 71182-26-8

L3 ANSWER 239 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 90:152149 CASREACT  
 TITLE: Studies on the synthesis of heterocyclic compounds.  
 Part II. Action of phosphorus oxychloride on  
 N-methyl-N-(1-phenyl-3-methylpyrazol-5-yl)-2-  
 acetamidobenzamide  
 AUTHOR(S): Plescia, S.; Daidone, G.; Sprio, V.; Aiello, E.;  
 Dattolo, G.; Cirrincione, G.  
 CORPORATE SOURCE: Ist. Chim. Farm., Univ. Studi Palermo, Palermo, Italy  
 SOURCE: Journal of Heterocyclic Chemistry (1978), 15(8),  
 1339-42  
 CODEN: JHTCAD; ISSN: 0022-152X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



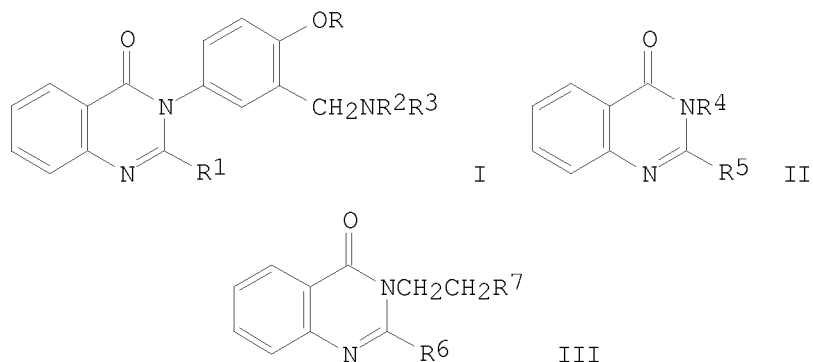
AB During attempts to prepare I by cyclization of II under Bischler-Napieralski reaction conditions, the formation of the macro-heterocycle III was observed

$$\text{RX}(4) \text{ OF } 12 \quad \dots \text{H} \implies \text{I}$$


RX (4)      RCT   H 69893-73-8  
              RGT   J 10025-87-3   POC13  
              PRO   I 65183-11-1

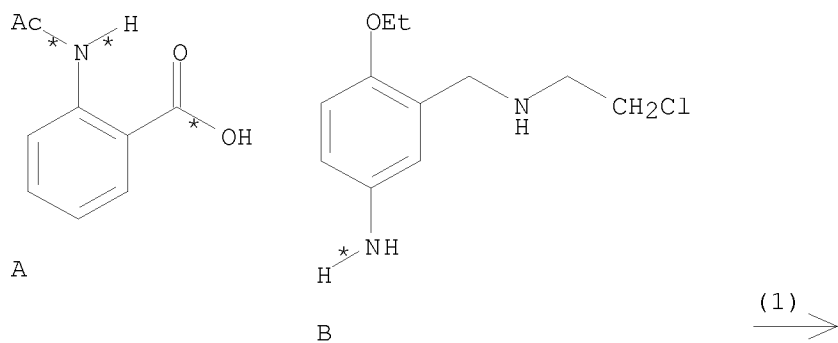
L3 ANSWER 240 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 90:152109 CASREACT  
TITLE: Study in nitrogen mustards. Part II. Synthesis of  
some 2-alkyl-3-aryl-4(3H)-quinazolinone derivatives as  
possible antitumor agents  
AUTHOR(S): Singh, Pritpal  
CORPORATE SOURCE: Dep. Chem. Eng. Technol., Panjab Univ., Chandigarh,  
India  
SOURCE: Journal of the Indian Chemical Society (1978), 55(8),  
801-5  
CODEN: JICSAH; ISSN: 0019-4522

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

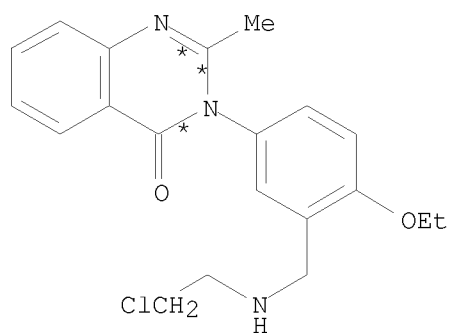


AB    Quinazolinone mustards I ( $R = H, Me, Et$ ;  $R_1 = H, Me$ ;  $R_2, R_3 = H, CH_2CH_2Cl, CH_2CH_2Br$ ) (25 compds.), II [ $R_4 = (ClCH_2CH_2)_2NC_6H_4SO_2, (HOCH_2CH_2)_2N, (ClCH_2CH_2)_2N, (BrCH_2CH_2)_2N, (ClCH_2CH_2)_2NC_6H_4$ ;  $R_5 = H, Me$ ] (9 compds.), and III [ $R_6 = H, Me$ ;  $R_7 = (HOCH_2CH_2)_2N, (ClCH_2CH_2)_2N, (BrCH_2CH_2)_2N, [(ClCH_2CH_2)_2NCH_2](R_8O)C_6H_3NH$  ( $R_8 = H, Me, Et$ )] (13 compds.) were prepared and possess activity against lymphoid leukemia L1210 in preliminary screening. Thus, cyclocondensation of 2-(AcNH) $C_6H_4CO_2Me$  with 2,5-(EtO)( $H_2N$ ) $C_6H_3CH_2N(CH_2CH_2Cl)_2$  gave 75% I ( $R = Et, R_1 = Me, R_2 = R_3 = ClCH_2CH_2$ ). Amination of III ( $R_6 = Me, R_7 = Cl$ ) with ( $BrCH_2CH_2$ ) $_2NH$  gave 80% III ( $R_6 = Me, R_7 = (BrCH_2CH_2)_2N$ ).

RX(1) OF 23            A + B ==> C



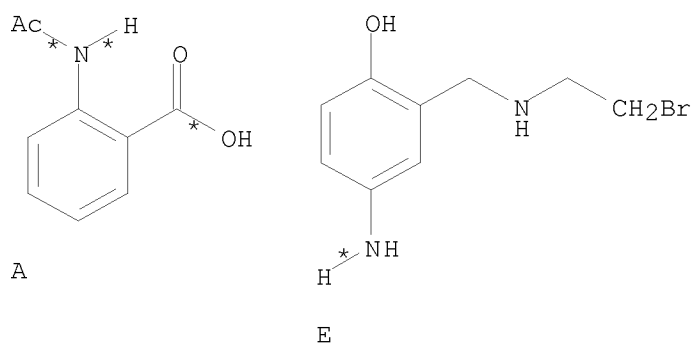
10/ 562,112



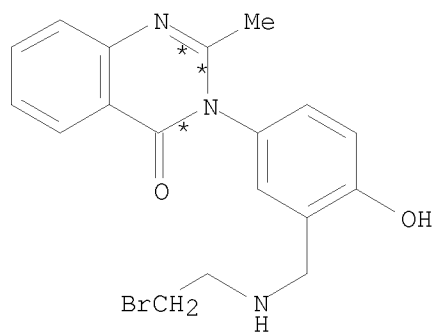
C  
YIELD 57%

RX(1) RCT A 89-52-1, B 56538-52-4  
RGT D 7789-60-8 PBr<sub>3</sub>  
PRO C 69561-23-5

RX(2) OF 23 A + E ==> F



(2)  $\longrightarrow$

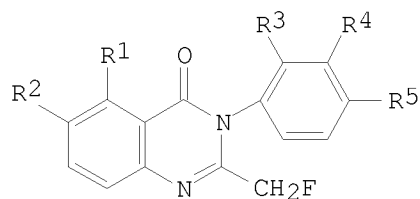


F  
YIELD 62%

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RX(2) RCT A 89-52-1, E 69561-59-7  
RGT D 7789-60-8 PBr3  
PRO F 69561-24-6

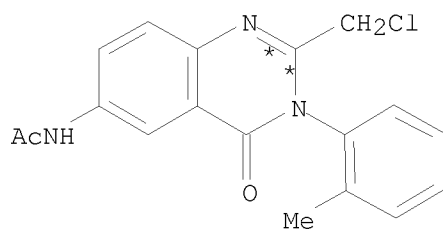
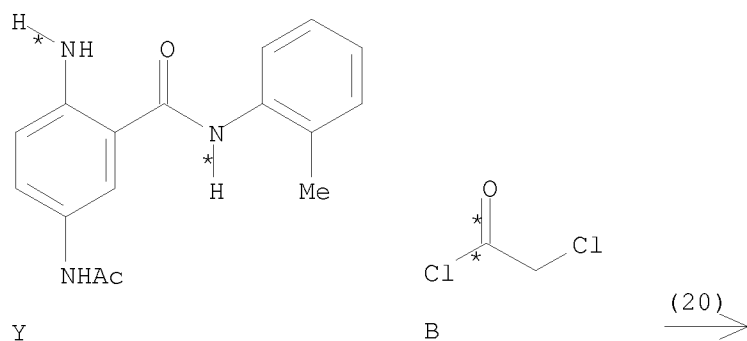
L3 ANSWER 241 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 90:80710 CASREACT  
TITLE: Studies on biologically active halogenated compounds.  
1. Synthesis and central nervous system depressant  
activity of 2-(fluoromethyl)-3-aryl-4(3H)-  
quinazolinone derivatives  
AUTHOR(S): Tani, Junichi; Yamada, Yoshihisa; Oine, Toyonari;  
Ochiai, Takashi; Ishida, Ryuichi; Inoue, Ichizo  
CORPORATE SOURCE: Res. Lab., Tanabe Seiyaku Co., Ltd., Osaka, Japan  
SOURCE: Journal of Medicinal Chemistry (1979), 22(1), 95-9  
CODEN: JMCMAR; ISSN: 0022-2623  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB The title compds. I (R1 = H or Cl; R2 = H, Cl, NH2, NO2 or NHAc; R3 = H, Cl, or Me; R4 and R5 = H or Cl) were prepared by the reaction of the appropriate anthranilic acid derivative with SOCl2 followed by treatment with anilines, chloroacetylation of the formed anthranilanilides and their cyclization followed by displacement of Cl by F. CNS activities of I were compared to methaqualone and 6-aminomethaqualone. 3-(3-Chloro-o-tolyl)-2-(fluoromethyl)-4-(3H)-quinazolinone [49700-31-4] was more potent in CNS depressant activity and less toxic than methaqualone. Structure-activity relations are discussed.

RX(20) OF 78 ...Y + B ==> AF...

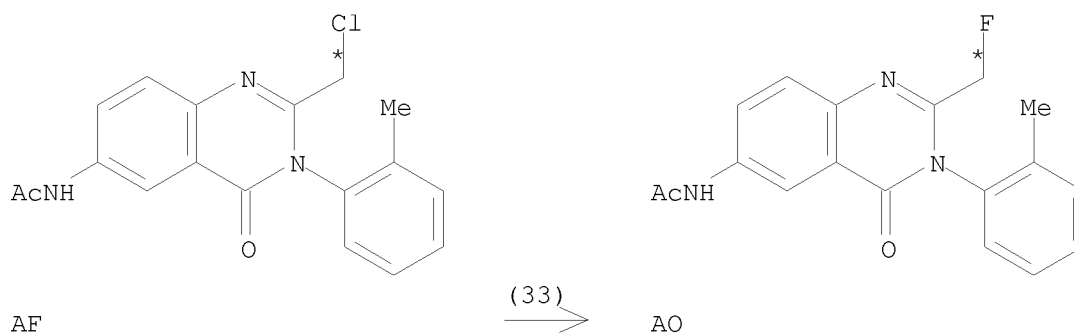
10/ 562,112



AF  
YIELD 81%

RX(20) RCT Y 64102-81-4, B 79-04-9  
PRO AF 61899-78-3

RX(33) OF 78 ...AF ==> AO...

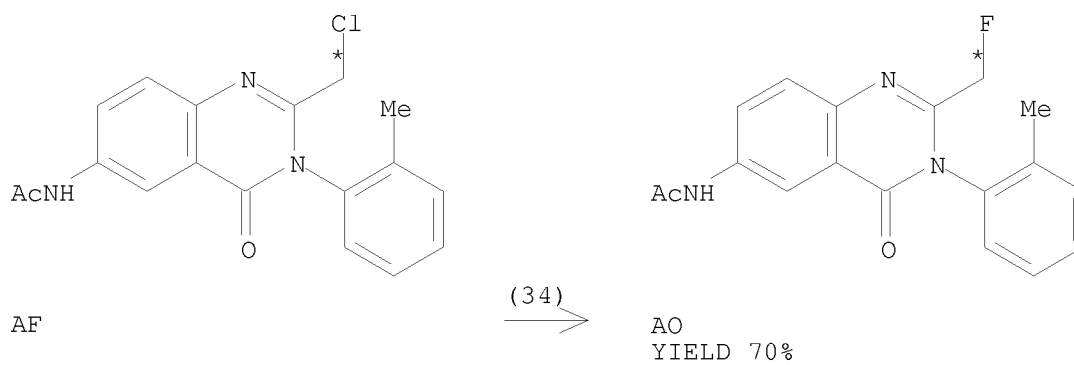


RX(33) RCT AF 61899-78-3  
RGT I 7789-23-3 KF  
PRO AO 61899-79-4

RX(34) OF 78 AF ==> AO

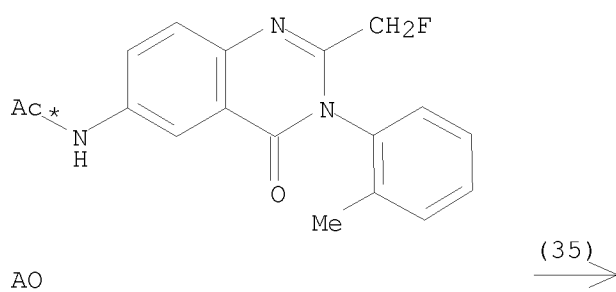


10/ 562,112



RX(34) RCT AF 61899-78-3  
PRO AO 61899-79-4

RX(35) OF 78 ...AO ==> AP

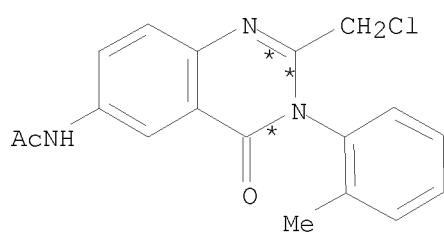
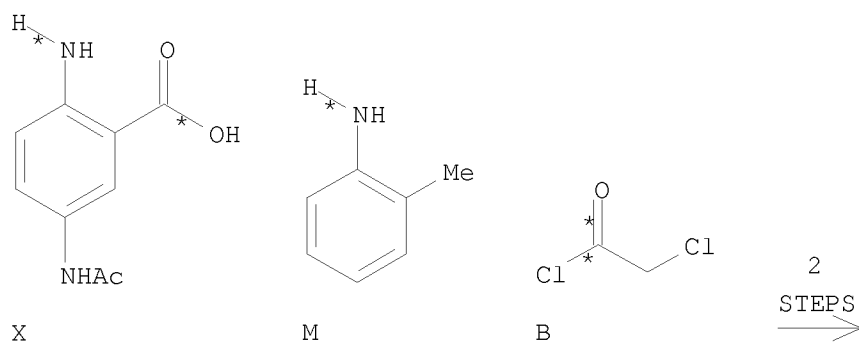


AP  
YIELD 61%

RX(35) RCT AO 61899-79-4  
PRO AP 56287-74-2

RX(51) OF 78 COMPOSED OF RX(13), RX(20)  
RX(51) X + M + B ==> AF

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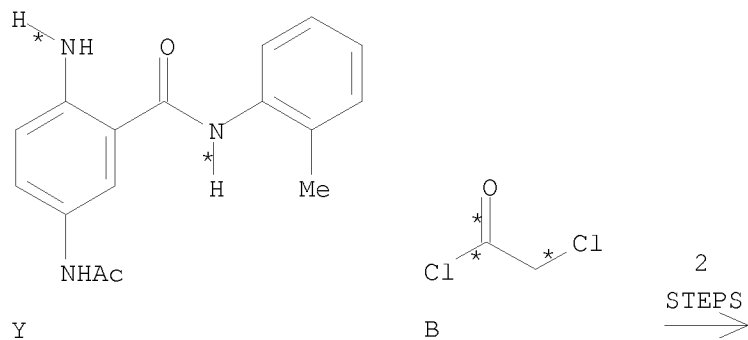


AF  
YIELD 81%

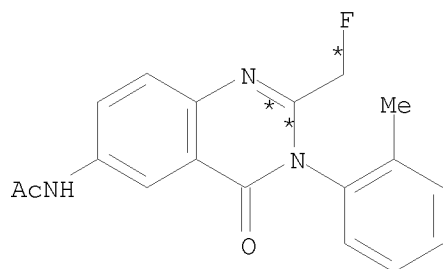
RX(13) RCT X 50670-83-2, M 95-53-4  
PRO Y 64102-81-4

RX(20) RCT Y 64102-81-4, B 79-04-9  
PRO AF 61899-78-3

RX(58) OF 78 COMPOSED OF RX(20), RX(33)  
RX(58) Y + B ==> AO



10/ 562,112

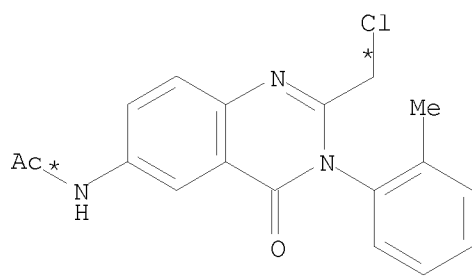


AO

RX(20) RCT Y 64102-81-4, B 79-04-9  
PRO AF 61899-78-3

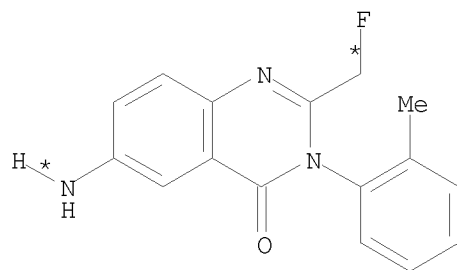
RX(33) RCT AF 61899-78-3  
RGT I 7789-23-3 KF  
PRO AO 61899-79-4

RX(60) OF 78 COMPOSED OF RX(33), RX(35)  
RX(60) AF ==> AP



AF

2  
STEPS  
→



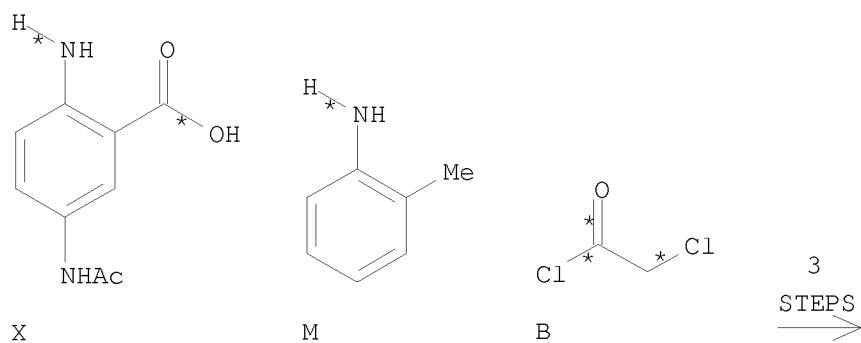
AP  
YIELD 61%

10/ 562,112

RX(33)      RCT    AF 61899-78-3  
              RGT    I 7789-23-3 KF  
              PRO    AO 61899-79-4

RX(35)      RCT    AO 61899-79-4  
              PRO    AP 56287-74-2

RX(72) OF 78 COMPOSED OF RX(13), RX(20), RX(33)  
RX(72)      X    +    M    +    B    ==>    AO



AO

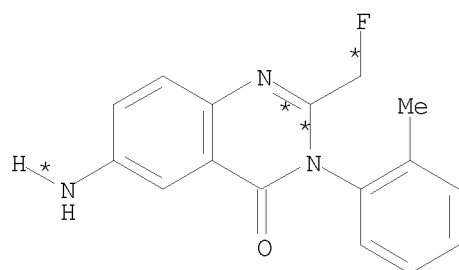
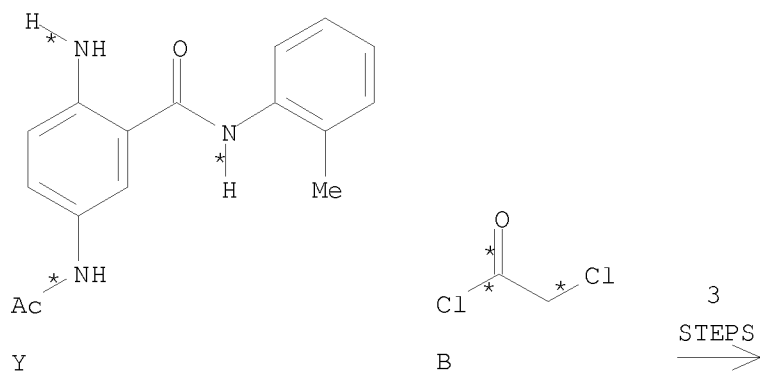
RX(13)      RCT    X 50670-83-2, M 95-53-4  
              PRO    Y 64102-81-4

RX(20)      RCT    Y 64102-81-4, B 79-04-9  
              PRO    AF 61899-78-3

RX(33)      RCT    AF 61899-78-3  
              RGT    I 7789-23-3 KF  
              PRO    AO 61899-79-4

RX(75) OF 78 COMPOSED OF RX(20), RX(33), RX(35)  
RX(75)      Y    +    B    ==>    AP

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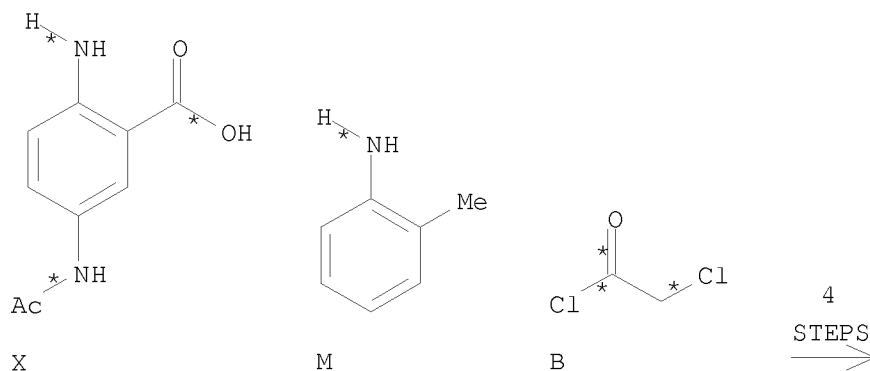
AP  
YIELD 61%

RX(20) RCT Y 64102-81-4, B 79-04-9  
PRO AF 61899-78-3

RX(33) RCT AF 61899-78-3  
RGT I 7789-23-3 KF  
PRO AO 61899-79-4

RX(35) RCT AO 61899-79-4  
PRO AP 56287-74-2

RX(76) OF 78 COMPOSED OF RX(13), RX(20), RX(33), RX(35)  
RX(76) X + M + B ==> AP



AP  
YIELD 61%

RX(13) RCT X 50670-83-2, M 95-53-4  
PRO Y 64102-81-4

RX(20) RCT Y 64102-81-4, B 79-04-9  
PRO AF 61899-78-3

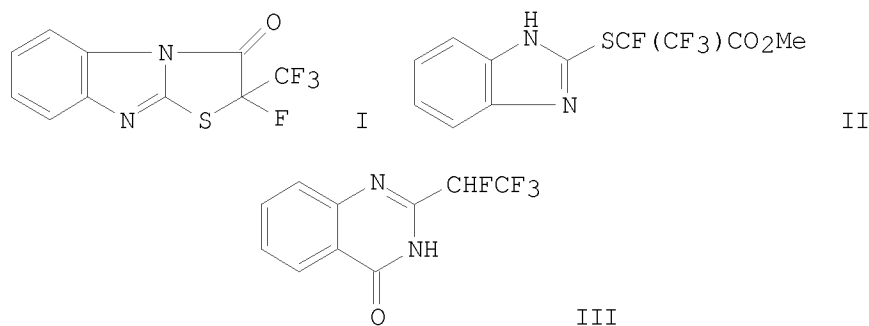
RX(33) RCT AF 61899-78-3  
RGT I 7789-23-3 KF  
PRO AO 61899-79-4

RX(35) RCT AO 61899-79-4  
PRO AP 56287-74-2

L3 ANSWER 242 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 90:38837 CASREACT  
TITLE: Preparation of fluorinated imidazole derivatives using  
hexafluoro-1,2-epoxypropane  
AUTHOR(S): Hammouda, Hamdy A.; Ishikawa, Nobuo  
CORPORATE SOURCE: Dep. Chem. Technol., Tokyo Inst. Technol., Tokyo,  
Japan  
SOURCE: Bulletin of the Chemical Society of Japan (1978),  
51(10), 3091-2

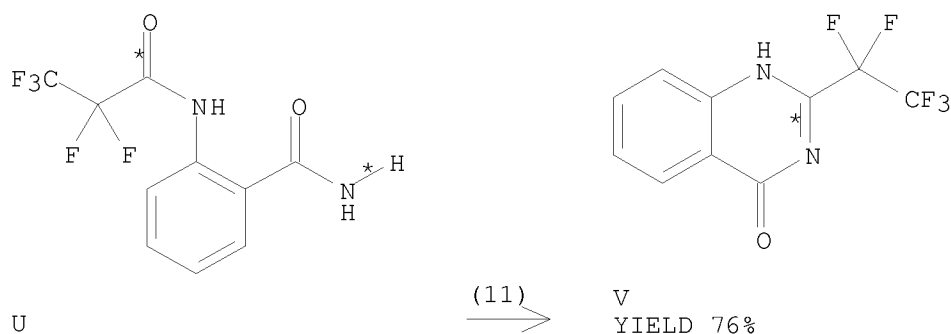
DOCUMENT TYPE:  
LANGUAGE:  
GI

CODEN: BCSJA8; ISSN: 0009-2673  
Journal  
English



AB Utilizing the reactivity of hexafluoro-1,2-epoxypropane, several new fluorine-containing imidazole derivs., e.g. I, II, and III, were prepared by reactions with 2-mercaptobenzimidazole, and o-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CONH<sub>2</sub>.

RX(11) OF 12 ...U ==> V



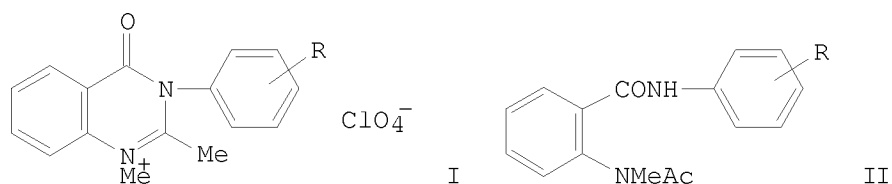
RX(11) RCT U 68790-62-5  
PRO V 35982-15-1

L3 ANSWER 243 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 89:43305 CASREACT  
TITLE: Study of 4(3H)-quinazolinones. IX. Synthesis and biological activity of 1,2-dimethyl-3-aryl-4(3H)-quinazolinonium perchlorates  
AUTHOR(S): Zalesov, V. S.; Kozhevnikov, Yu. V.; Pilat, V. S.; Gradel, I. I.  
CORPORATE SOURCE: Perm. Farm. Inst., Perm., USSR  
SOURCE: Izuch. Biol. Deistviya Nov. Prod. Org. Sint. Prir. Soedin. (1977), 131-6. Editor(s): Pidemskii, E. L. Permsk. Gos. Univ. im. A. M. Gor'kogo: Perm, USSR.

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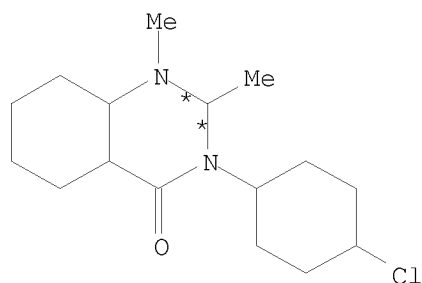
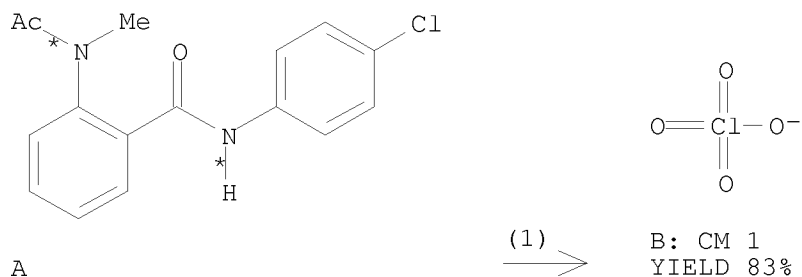
DOCUMENT TYPE:  
LANGUAGE:  
GI

CODEN: 37YKA4  
Conference  
Russian



AB The title compds. I (R = H, 2-, 3-, 4-Me, 2-, 4-Cl, 2-, 3-, 4-Br, 4-MeO, 4-EtO), useful as antispasmodics, were prepared in 64-90% yields by cyclization of II, prepared in 48-80% yields by acetylation of the corresponding amine, with HClO<sub>4</sub>.

RX(1) OF 11 A ==> B

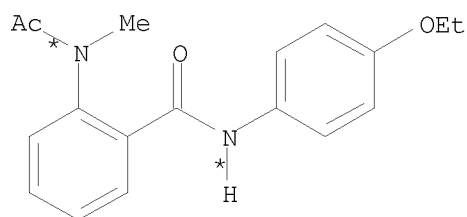


B: CM 2  
YIELD 83%

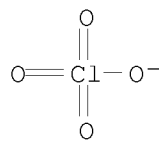
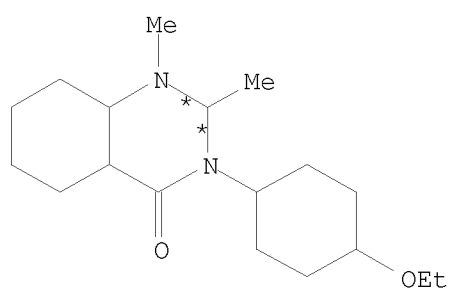
RX(1) RCT A 66860-37-5  
RGT C 7601-90-3 HClO<sub>4</sub>  
PRO B 66860-54-6

RX(2) OF 11 D ==> E



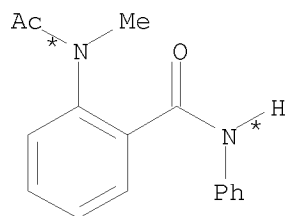


D

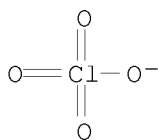
(2)  $\longrightarrow$ E: CM 1  
YIELD 74%E: CM 2  
YIELD 74%

RX(2)      RCT   D 66860-42-2  
              RGT   C 7601-90-3 HClO4  
              PRO   E 66860-63-7

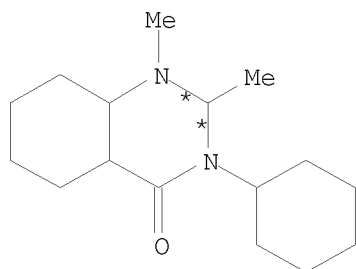
RX(3) OF 11      F    ==&gt;    G



F

(3)  $\longrightarrow$ G: CM 1  
YIELD 65%

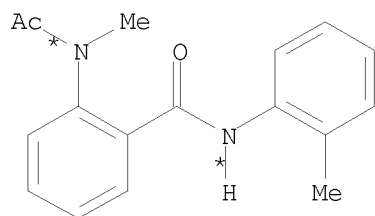
10/ 562,112



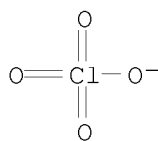
G: CM 2  
YIELD 65%

RX(3)      RCT    F 66860-32-0  
              RGT    C 7601-90-3 HClO4  
              PRO    G 66860-44-4

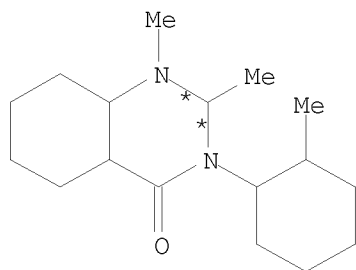
RX(4) OF 11      H    ==>    I



H



I: CM 1  
YIELD 74%

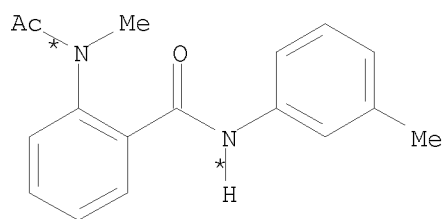


I: CM 2  
YIELD 74%

RX(4)      RCT    H 66860-33-1  
              RGT    C 7601-90-3 HClO4  
              PRO    I 66860-46-6

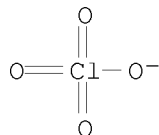
10/ 562,112

RX(5) OF 11 J ==> K

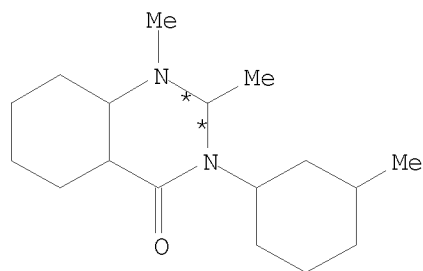


J

(5)  $\longrightarrow$



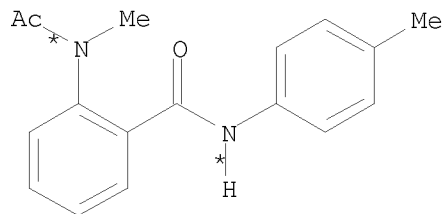
K: CM 1  
YIELD 60%



K: CM 2  
YIELD 60%

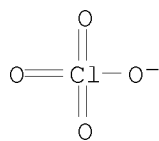
RX(5) RCT J 66860-34-2  
RGT C 7601-90-3 HClO<sub>4</sub>  
PRO K 66860-48-8

RX(6) OF 11 L ==> M



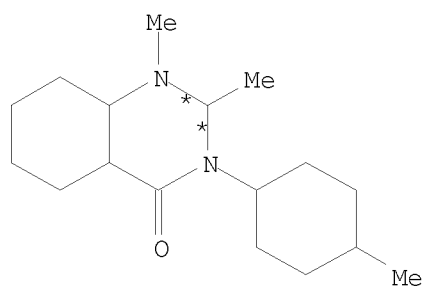
L

(6)  $\longrightarrow$



M: CM 1  
YIELD 80%

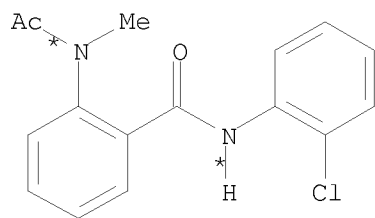
10/ 562,112



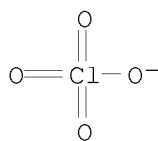
M: CM 2  
YIELD 80%

RX(6)        RCT    L 66860-35-3  
              RGT    C 7601-90-3 HClO4  
              PRO    M 66860-50-2

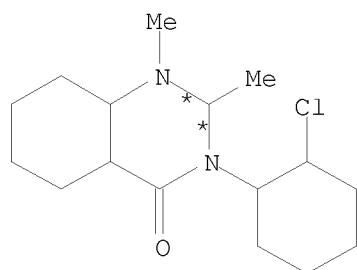
RX(7) OF 11        N    ==>    O



N



O: CM 1  
YIELD 58%

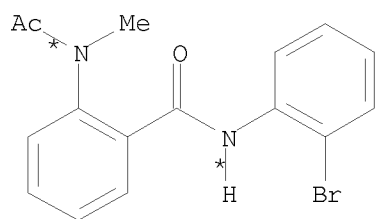


O: CM 2  
YIELD 58%

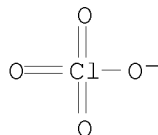
RX(7)        RCT    N 66860-36-4  
              RGT    C 7601-90-3 HClO4  
              PRO    O 66860-52-4

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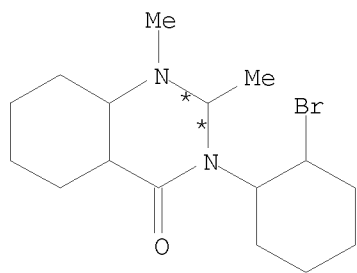
RX(8) OF 11 P ==> Q



P



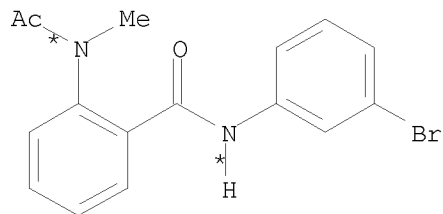
Q: CM 1  
YIELD 64%



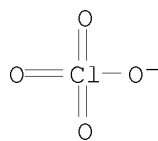
Q: CM 2  
YIELD 64%

RX(8) RCT P 66860-38-6  
RGT C 7601-90-3 HClO4  
PRO Q 66860-55-7

RX(9) OF 11 R ==> S

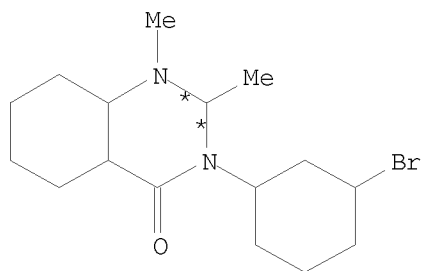


R



S: CM 1  
YIELD 70%

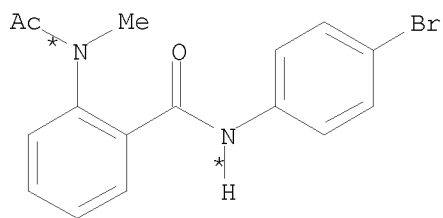
10/ 562,112



S: CM 2  
YIELD 70%

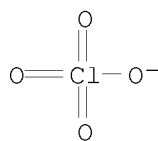
RX(9)        RCT    R 66860-39-7  
              RGT    C 7601-90-3 HClO4  
              PRO    S 66860-57-9

RX(10) OF 11        T    ==>    U

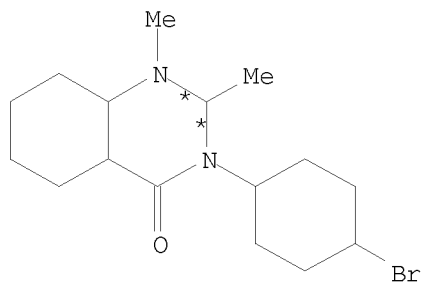


T

(10)  $\Rightarrow$



U: CM 1  
YIELD 90%

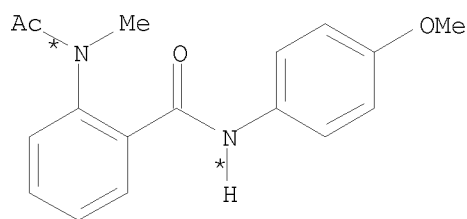


U: CM 2  
YIELD 90%

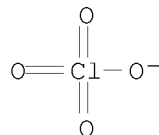
RX(10)        RCT    T 66860-40-0  
              RGT    C 7601-90-3 HClO4  
              PRO    U 66860-59-1

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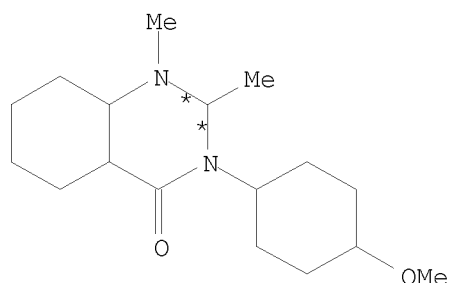
RX(11) OF 11 V ==> W



V



W: CM 1  
YIELD 85%

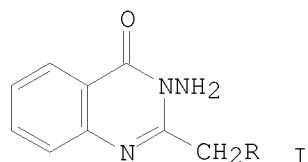


W: CM 2  
YIELD 85%

RX(11) RCT V 66860-41-1  
RGT C 7601-90-3 HClO4  
PRO W 66860-61-5

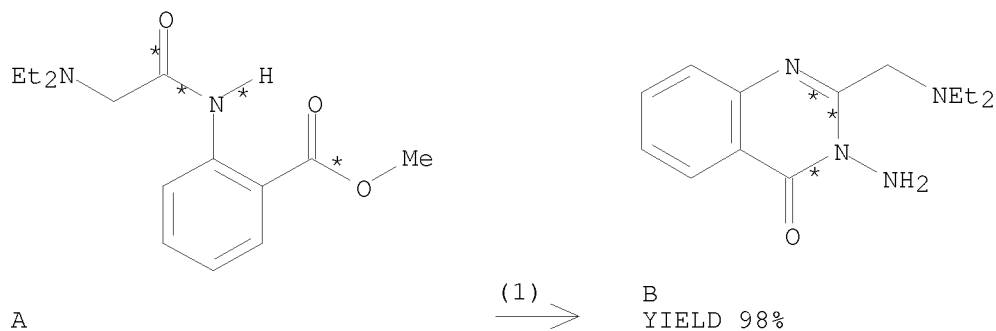
L3 ANSWER 244 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 87:201459 CASREACT  
TITLE: New 3-aminoquinazolinones  
AUTHOR(S): Sauter, Fritz; Stanetty, Peter; Jordis, Ulrich  
CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Wien, Vienna, Austria  
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1977),  
310(8), 680-2  
CODEN: ARPMAS; ISSN: 0365-6233  
DOCUMENT TYPE: Journal  
LANGUAGE: German  
GI

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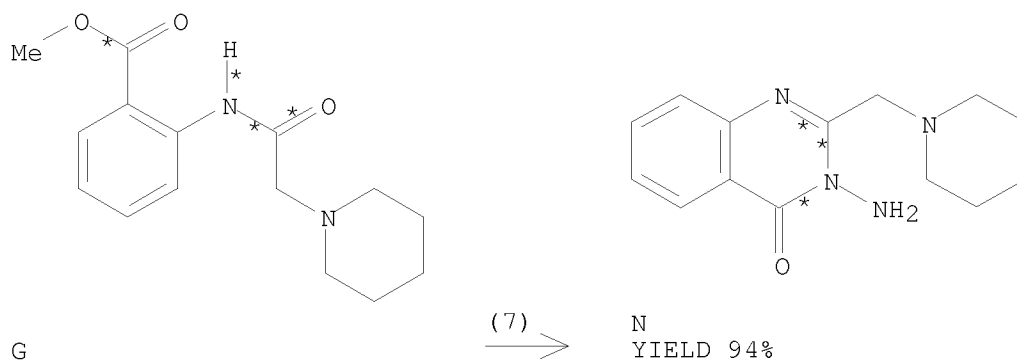
AB Aminoquinazolinones I (R = NEt<sub>2</sub>, piperidino, 2,6-dimethylpiperidino, morpholino, 4-methyl-1-piperazinyl) were obtained in 47-98% yield by treating 2-MeO<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>NHCOCH<sub>2</sub>R (II: R as above) with N<sub>2</sub>H<sub>4</sub>. II (R = amino) were obtained by chloroacetylating Me anthranilate, iodinating II (R = Cl), and aminating II (R = I).

RX(1) OF 15 ...A ==> B



RX(1) RCT A 64689-29-8  
RGT C 302-01-2 N<sub>2</sub>H<sub>4</sub>  
PRO B 64689-30-1

RX(7) OF 15 ...G ==> N



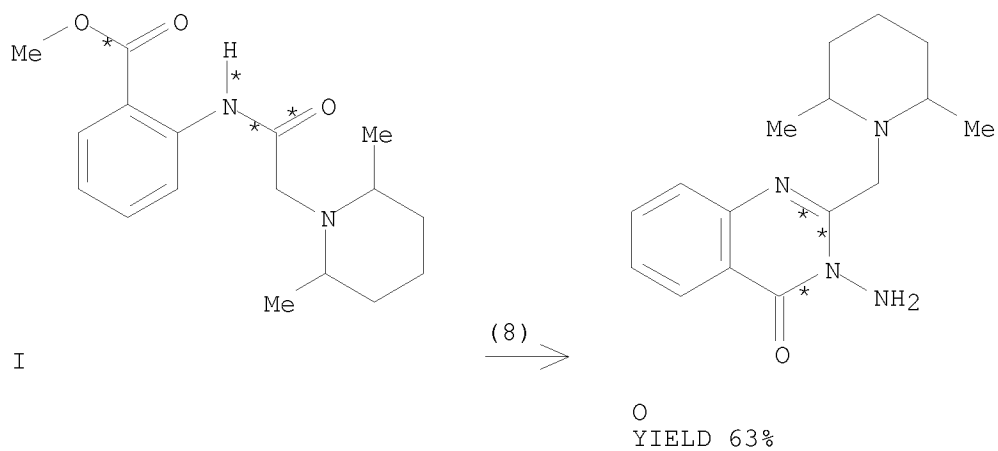
RX(7) RCT G 64689-25-4



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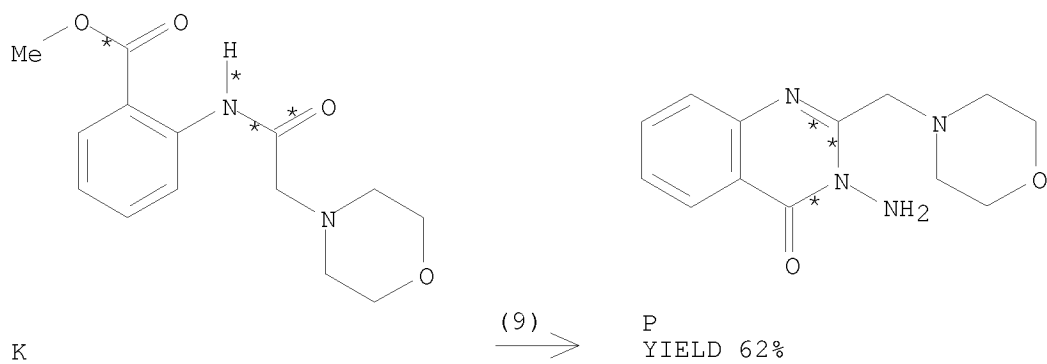
RGT C 302-01-2 N2H4  
PRO N 64689-31-2

RX(8) OF 15 ...I ==> O



RX(8) RCT I 64689-26-5  
RGT C 302-01-2 N2H4  
PRO O 64689-32-3

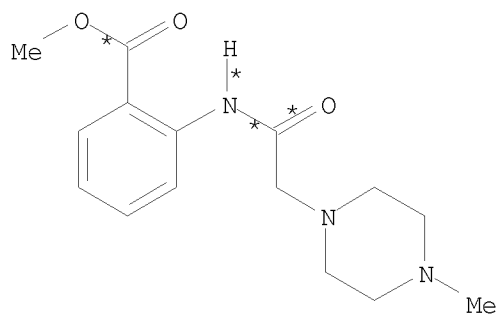
RX(9) OF 15 ...K ==> P



RX(9) RCT K 64689-27-6  
RGT C 302-01-2 N2H4  
PRO P 64689-33-4

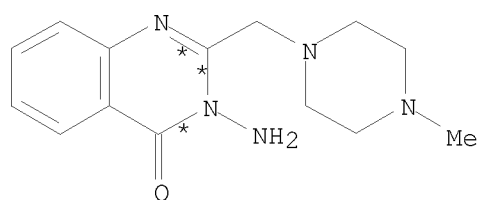
RX(10) OF 15 ...M ==> Q

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M

(10)  $\longrightarrow$

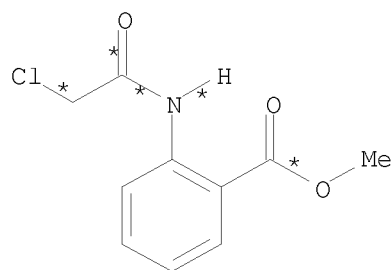


Q

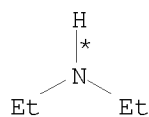
YIELD 47%

RX(10)      RCT    M 342414-65-7  
                  RGT    C 302-01-2 N2H4  
                  PRO    Q 64689-34-5

RX(11) OF 15 COMPOSED OF RX(2), RX(1)  
 RX(11)      D    +    E    ==>    B



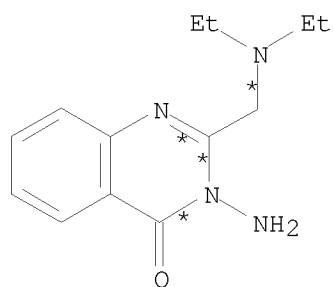
D



E

2  
 STEPS  $\longrightarrow$

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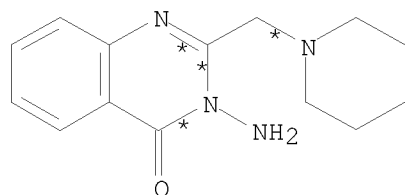
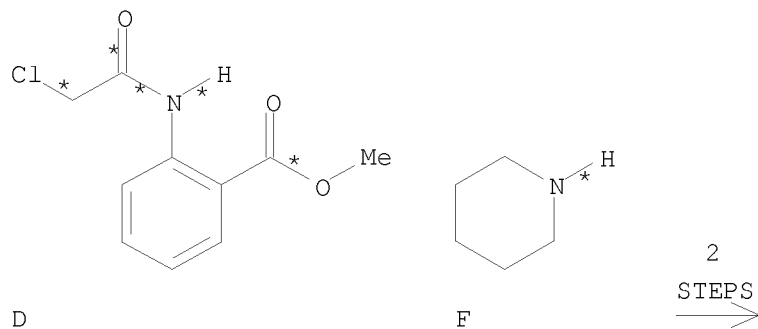


B  
YIELD 98%

RX(2) RCT D 58915-18-7, E 109-89-7  
PRO A 64689-29-8

RX(1) RCT A 64689-29-8  
RGT C 302-01-2 N2H4  
PRO B 64689-30-1

RX(12) OF 15 COMPOSED OF RX(3), RX(7)  
RX(12) D + F ==> N



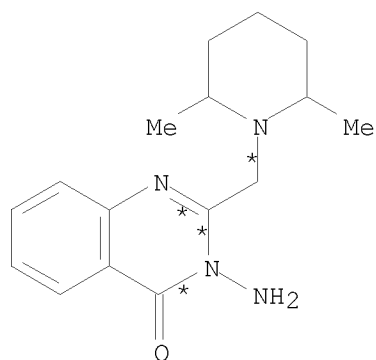
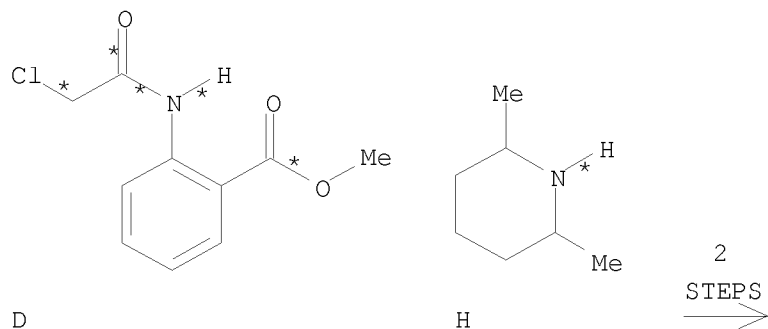
N  
YIELD 94%

RX(3) RCT D 58915-18-7, F 110-89-4  
PRO G 64689-25-4

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RX(7)        RCT    G 64689-25-4  
              RGT    C 302-01-2 N2H4  
              PRO    N 64689-31-2

RX(13) OF 15 COMPOSED OF RX(4), RX(8)  
RX(13)       D    +    H    ==>    O



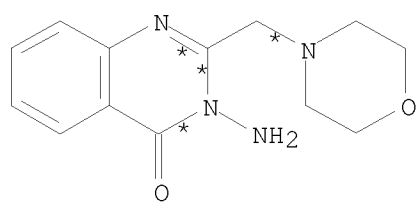
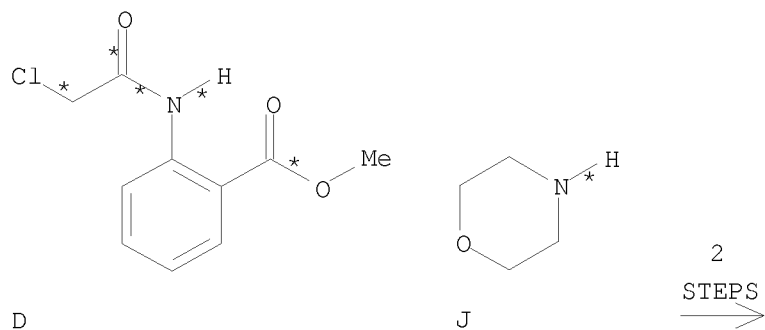
O  
YIELD 63%

RX(4)        RCT    D 58915-18-7, H 504-03-0  
              PRO    I 64689-26-5

RX(8)        RCT    I 64689-26-5  
              RGT    C 302-01-2 N2H4  
              PRO    O 64689-32-3

RX(14) OF 15 COMPOSED OF RX(5), RX(9)  
RX(14)       D    +    J    ==>    P

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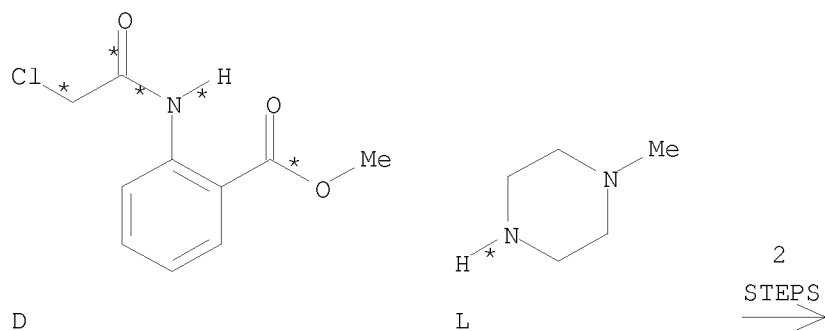


P  
YIELD 62%

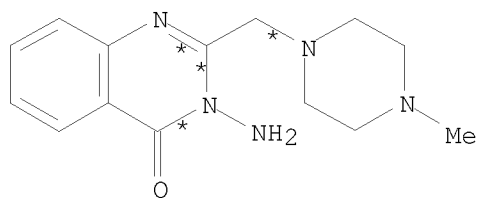
RX(5) RCT D 58915-18-7, J 110-91-8  
PRO K 64689-27-6

RX(9) RCT K 64689-27-6  
RGT C 302-01-2 N2H4  
PRO P 64689-33-4

RX(15) OF 15 COMPOSED OF RX(6), RX(10)  
RX(15) D + L ==> Q



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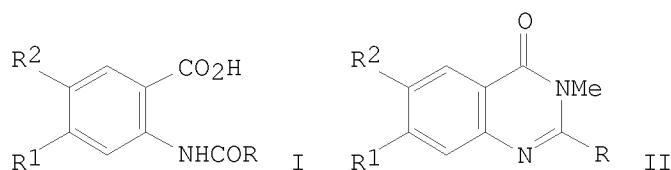


Q  
YIELD 47%

RX(6) RCT D 58915-18-7, L 109-01-3  
PRO M 342414-65-7

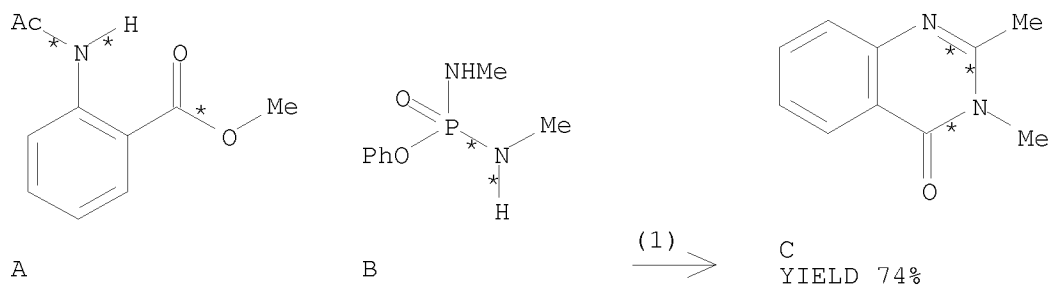
RX(10) RCT M 342414-65-7  
RGT C 302-01-2 N2H4  
PRO Q 64689-34-5

L3 ANSWER 245 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 87:39404 CASREACT  
TITLE: Phosphoramides; III. Phenyl  
N,N'-dimethylphosphorodiamidate as a new reagent for  
the synthesis of  
3-methyl-4-oxo-3,4-dihydroquinazolines  
AUTHOR(S): Pedersen, E. B.  
CORPORATE SOURCE: Dep. Chem., Odense Univ., Odense, Den.  
SOURCE: Synthesis (1977), (3), 180-1  
CODEN: SYNTBF; ISSN: 0039-7881  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



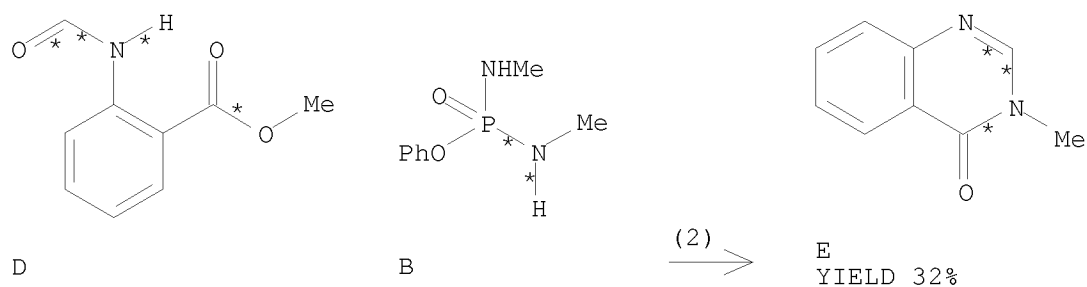
AB Treatment of the acylantranilates I (R = H, Me, Et, Ph; R1, R2 = H, Me, MeO) with PhOP(O)(NHMe)2 at 250° gave the quinazolinones II in 32-74% yields.

RX(1) OF 6 A + B ==> C



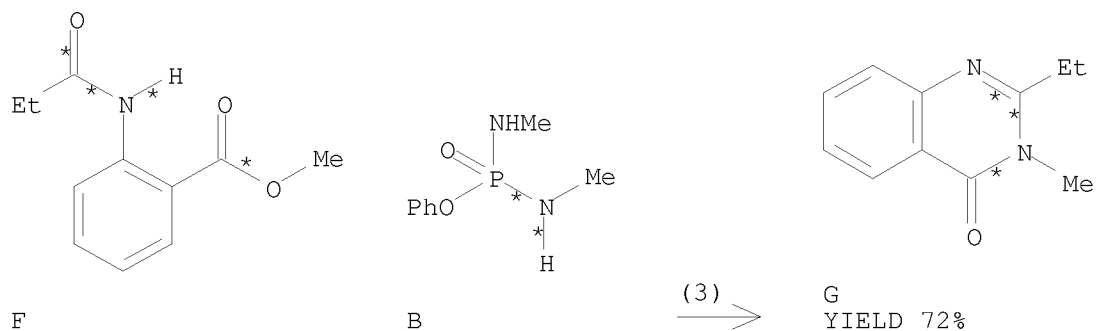
RX(1) RCT A 2719-08-6, B 1754-58-1  
PRO C 1769-25-1

RX(2) OF 6 D + B ==> E



RX(2) RCT D 41270-80-8, B 1754-58-1  
PRO E 2436-66-0

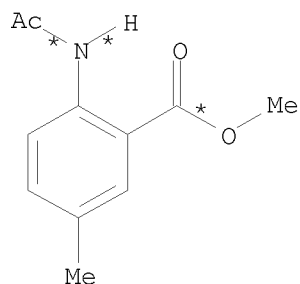
RX(3) OF 6 F + B ==> G



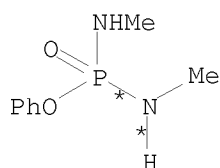
RX(3) RCT F 25628-84-6, B 1754-58-1  
PRO G 58718-53-9

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RX(5) OF 6 J + B ==> K

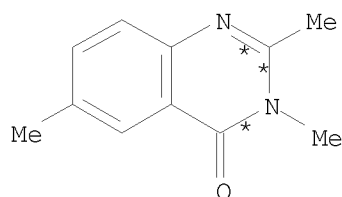


J



B

(5)  $\longrightarrow$



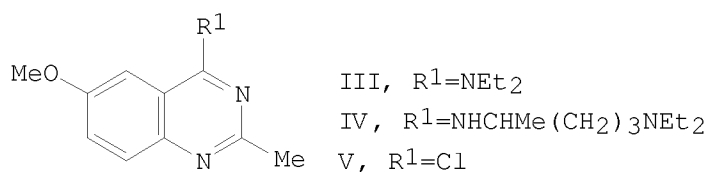
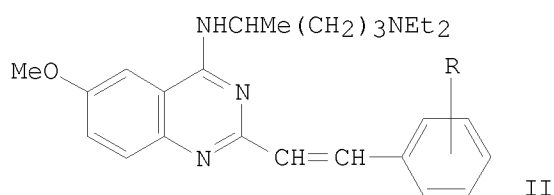
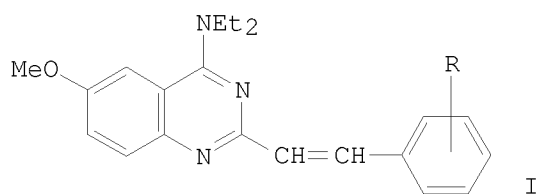
K

YIELD 40%

RX(5) RCT J 37619-22-0, B 1754-58-1  
PRO K 63190-58-9

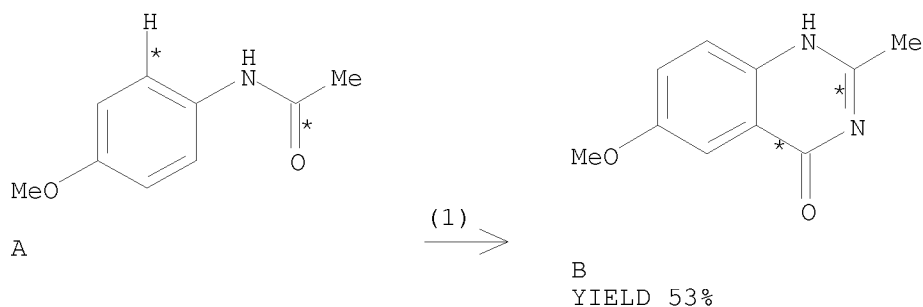
L3 ANSWER 246 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 85:123848 CASREACT  
TITLE: Synthesis and chemotherapeutic study of substituted  
2-styryl-4-amino-6-methoxyquinazolines  
AUTHOR(S): Zhikhareva, G. P.; Pronina, E. V.; Golovanova, E. A.;  
Pershin, G. N.; Novitskaya, N. A.; Zykova, T. N.;  
Gus'kova, T. A.; Yakhontov, L. N.  
CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst. im.  
Ordzhonikidze, Moscow, USSR  
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1976), 10(4), 62-6  
CODEN: KHFZAN; ISSN: 0023-1134  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
GI





AB The quinazolines I and II (R = o-Cl, p-Cl, p-Br, o-NO<sub>2</sub>, p-NO<sub>2</sub>) were prepared in 18-65% yield by condensation of III and IV, resp., with RC<sub>6</sub>H<sub>4</sub>CHO. III and IV were prepared by reaction of p-MeOC<sub>6</sub>H<sub>4</sub>NHAc with H<sub>2</sub>NCO<sub>2</sub>Et to give 53% 6-methoxy-2-methyl-4-quinazolone; this was converted to V, which was treated with Et<sub>2</sub>NH and H<sub>2</sub>NCHMe(CH<sub>2</sub>)<sub>3</sub>NEt<sub>2</sub>, resp. II (R = o-Cl) has min. inhibitory concentration of 4-30 µg/ml against gram-pos. bacteria; I (R = o-Cl) and II (R = o-Cl, o-NO<sub>2</sub>) have min. inhibitory concns. of 0.5-8 µg/ml against tuberculosis mycobacteria. The growth of fungi was inhibited only at high concns.

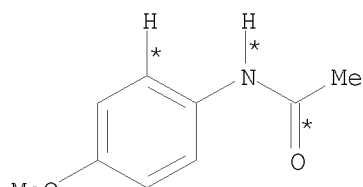
RX(1) OF 9 A ==> B...



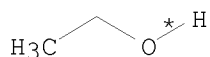
RX(1) RCT A 51-66-1  
PRO B 51413-71-9

RX(9) OF 9 COMPOSED OF RX(1), RX(2), RX(4)  
RX(9) A + G ==> H

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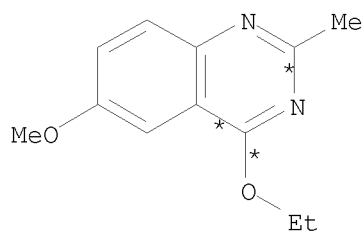


A



G

3  
STEPS  
→



● HCl

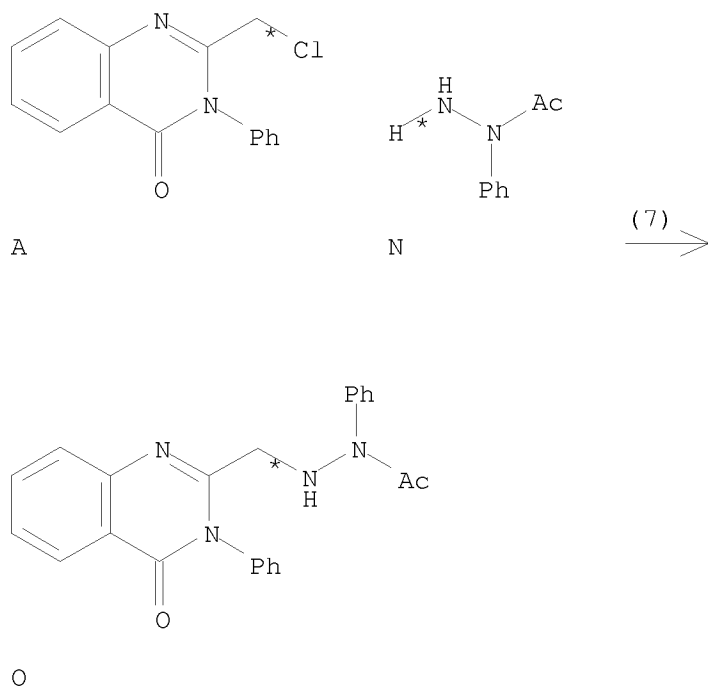
H

YIELD 82%

RX(1)	RCT	A 51-66-1
	PRO	B 51413-71-9
RX(2)	RCT	B 51413-71-9
	RGT	D 10025-87-3 POC13
	PRO	C 60395-90-6
RX(4)	RCT	C 60395-90-6, G 64-17-5
	PRO	H 60395-91-7
	SOL	64-17-5 EtOH

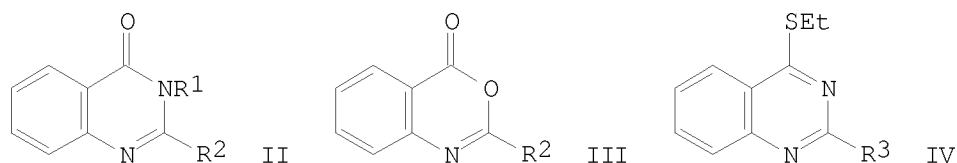
L3 ANSWER 247 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 85:46575 CASREACT  
TITLE: Studies on 4-quinazolone. IV. Synthesis and properties of 2-(β-phenylhydrazinomethyl)-3-aryl-4-quinazolones  
AUTHOR(S): Kozhevnikov, Yu. V.  
CORPORATE SOURCE: USSR  
SOURCE: Nauch. Tr. Perm. Farmatsevt. In-t (1975), (8), 35-7  
From: Ref. Zh., Khim. 1976, Abstr. No. 9Zh276  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
AB Title only translated.

RX (7) OF 11 A + N ==&gt; 0



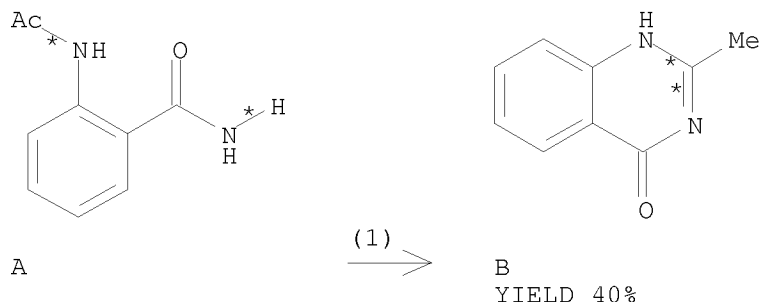
RX(7) RCT A 22312-77-2, N 2116-41-8  
PRO O 60431-83-6

```
L3      ANSWER 248 OF 258      CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:              85:21282  CASREACT
TITLE:                          Reaction of triethyloxonium fluoroborate with acid
                                amide.  III.  Formation of quinazoline and
                                4H-3,1-benzoxazin-4-one derivatives
AUTHOR(S):                     Kato, Takehiko; Takada, Atsushi; Ueda, Takeo
CORPORATE SOURCE:              Sch. Pharm. Sci., Kitasato Univ., Tokyo, Japan
SOURCE:                         Chemical & Pharmaceutical Bulletin (1976), 24(3),
                                431-6
                                CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE:                  Journal
LANGUAGE:                       English
GI
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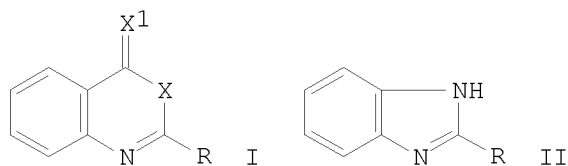
AB Reaction of o-R<sub>1</sub>NHCO C<sub>6</sub>H<sub>4</sub>NHCOR<sub>2</sub> (I, R<sub>1</sub> = H, Me, Et, Pr, Ph, o-C<sub>6</sub>H<sub>4</sub>Me, -C<sub>6</sub>H<sub>4</sub>OMe, -C<sub>6</sub>H<sub>4</sub>OEt, CH<sub>2</sub>Ph; R<sub>2</sub> = Me, Et, Pr, CHMe<sub>2</sub>) with Et<sub>3</sub>O<sup>+</sup>BF<sub>4</sub><sup>-</sup> gave the quinazolinones II, whereas I (R<sub>1</sub> = H, R<sub>2</sub> = Ph, o-, p-tolyl, p-C<sub>6</sub>H<sub>4</sub>OMe, o-, p-C<sub>6</sub>H<sub>4</sub>Cl) gave the quinoxazinones III and o-H<sub>2</sub>NC(S)C<sub>6</sub>H<sub>4</sub>NHCOR<sub>3</sub> (R<sub>3</sub> = Ph, Me, Et, p-C<sub>6</sub>H<sub>4</sub>R<sub>4</sub>, R<sub>4</sub> = Me, OMe, Cl, NO<sub>2</sub>), the quinazolines IV.

RX(1) OF 1 A ==> B



RX(1) RCT A 33809-77-7  
RGT C 368-39-8 Et<sub>3</sub>O.BF<sub>4</sub>  
PRO B 1769-24-0  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
NTE Classification: Condensation; Heterocycle formation;  
Cyclisation; Isomerisation; # Conditions: Et<sub>3</sub>O.BF<sub>4</sub> CH<sub>2</sub>Cl<sub>2</sub>; Rf 1h

L3 ANSWER 249 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 84:135575 CASREACT  
TITLE: Condensation reactions between o-phenylenediamine and  
2-substituted 1,3-benzoxazin-4-ones  
AUTHOR(S): Rabilloud, Guy; Sillion, Bernard  
CORPORATE SOURCE: Inst. Fr. Pet., CEN, Grenoble, Fr.  
SOURCE: Bulletin de la Societe Chimique de France (1975),  
(11-12, Pt. 2), 2682-6  
CODEN: BSCFAS; ISSN: 0037-8968  
DOCUMENT TYPE: Journal  
LANGUAGE: French  
GI

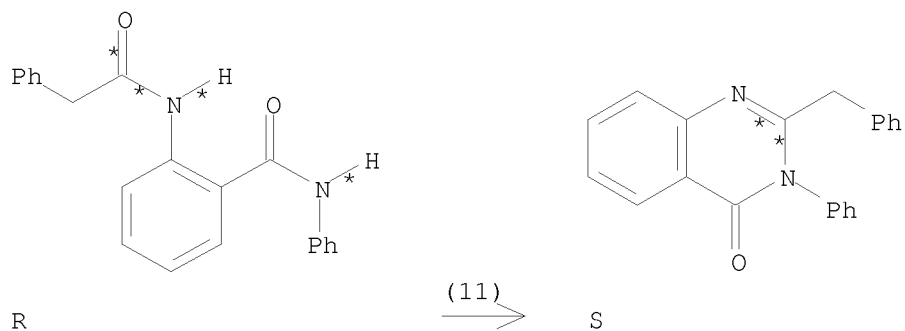


AB Condensation of benzoxazinones I (X = X<sub>1</sub> = O, R = Me, CH<sub>2</sub>Ph, Ph, Bz) with

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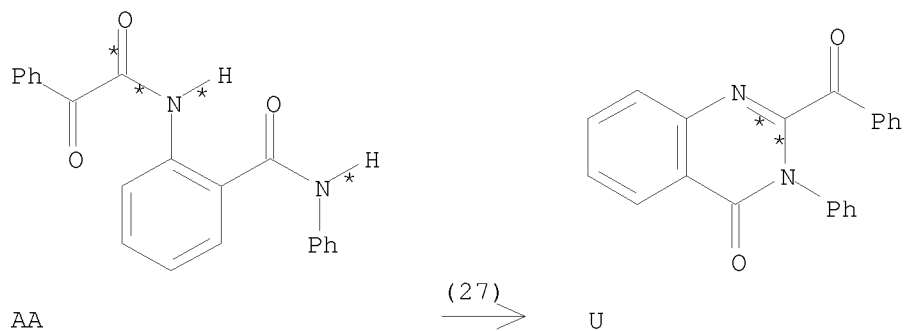
o-(H<sub>2</sub>N)<sub>2</sub>C<sub>6</sub>H<sub>4</sub> gave the benzimidazoles II (R = Me, CH<sub>2</sub>Ph, Ph, 2-PhCH<sub>2</sub>COC<sub>6</sub>H<sub>4</sub>), I (XX1 = o-NC<sub>6</sub>H<sub>4</sub>N:, R = CH<sub>2</sub>Ph, Ph), I (X1 = O, XR = o-NC<sub>6</sub>H<sub>4</sub>N:CPh) and 2-(2-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>NHCO)C<sub>6</sub>H<sub>4</sub>NHBz. Reaction of I (X = X1 = O, R = CH<sub>2</sub>Ph, Bz) with PhNH<sub>2</sub> gave I (X = NPh, X1 = O).

RX(11) OF 73 ...R ==> S...



RX(11) RCT R 74772-50-2  
 PRO S 19857-34-2  
 CAT 108-39-4 3-Methylphenol

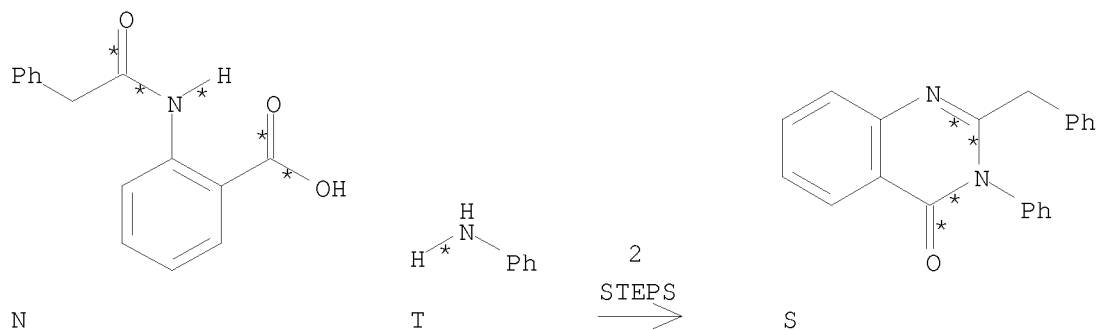
RX(27) OF 73 ...AA ==> U



RX(27) RCT AA 341545-11-7  
 PRO U 58980-14-6  
 CAT 108-39-4 3-Methylphenol

RX(33) OF 73 COMPOSED OF RX(9), RX(12)  
 RX(33) N + T ==> S

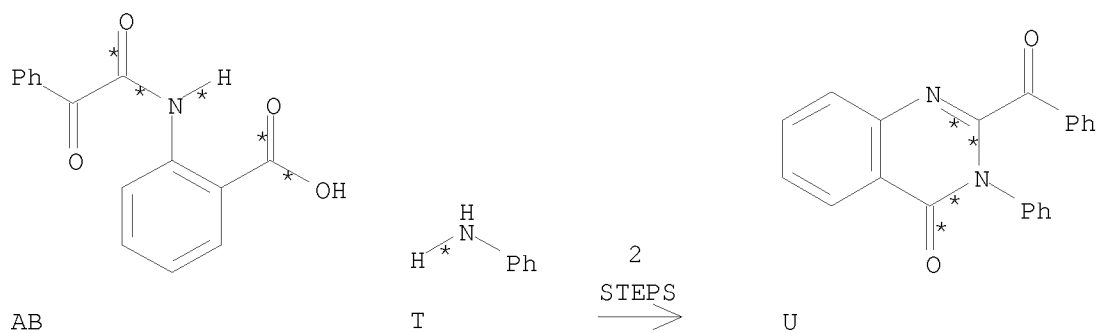
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RX(9) RCT N 28565-98-2  
PRO J 58980-13-5  
CAT 108-24-7 Ac2O

RX(12) RCT J 58980-13-5, T 62-53-3  
PRO S 19857-34-2  
CAT 108-39-4 3-Methylphenol

RX(40) OF 73 COMPOSED OF RX(26), RX(14)  
RX(40) AB + T ==> U

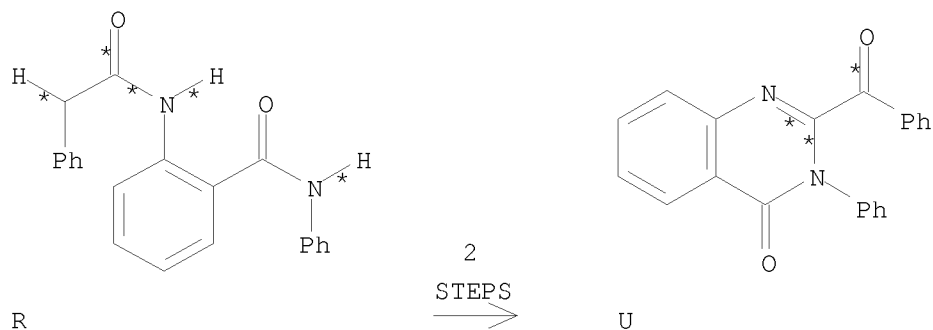


RX(26) RCT AB 58980-12-4  
PRO P 28565-99-3  
CAT 108-24-7 Ac2O

RX(14) RCT P 28565-99-3, T 62-53-3  
PRO U 58980-14-6  
CAT 108-39-4 3-Methylphenol

RX(43) OF 73 COMPOSED OF RX(11), RX(13)  
RX(43) R ==> U

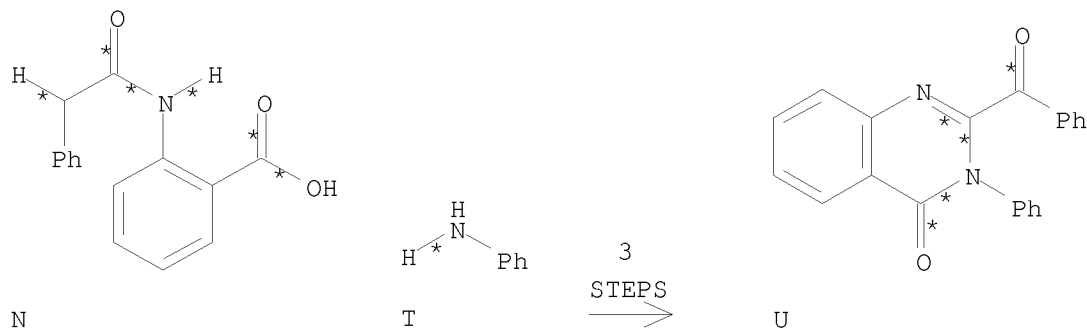
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RX(11)     RCT   R 74772-50-2  
              PRO   S 19857-34-2  
              CAT   108-39-4 3-Methylphenol

RX(13)     RCT   S 19857-34-2  
              RGT   Q 7446-08-4 SeO2  
              PRO   U 58980-14-6  
              CAT   108-24-7 Ac2O

RX(55) OF 73 COMPOSED OF RX(9), RX(10), RX(14)  
 RX(55)     N   +   T   ==>   U



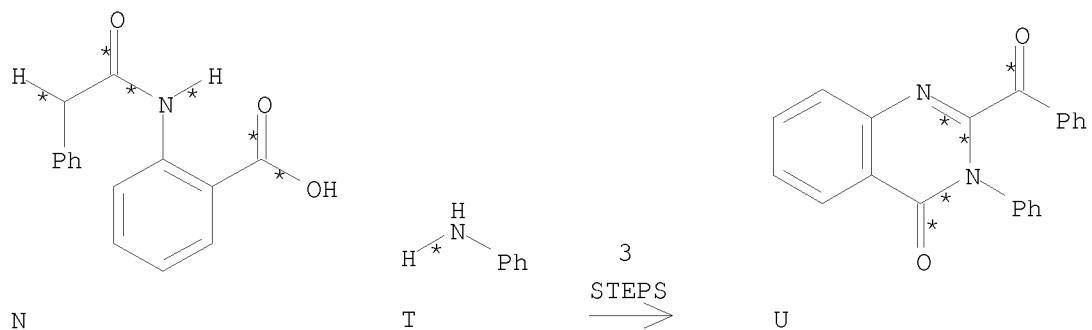
RX(9)       RCT   N 28565-98-2  
              PRO   J 58980-13-5  
              CAT   108-24-7 Ac2O

RX(10)     RCT   J 58980-13-5  
              RGT   Q 7446-08-4 SeO2  
              PRO   P 28565-99-3  
              CAT   108-24-7 Ac2O

RX(14)     RCT   P 28565-99-3, T 62-53-3  
              PRO   U 58980-14-6  
              CAT   108-39-4 3-Methylphenol

RX(58) OF 73 COMPOSED OF RX(9), RX(12), RX(13)  
 RX(58)     N   +   T   ==>   U

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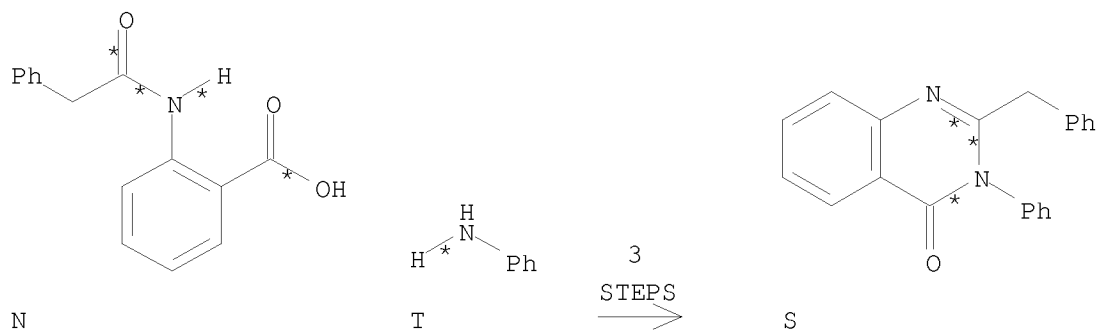


RX(9) RCT N 28565-98-2  
PRO J 58980-13-5  
CAT 108-24-7 Ac2O

RX(12) RCT J 58980-13-5, T 62-53-3  
PRO S 19857-34-2  
CAT 108-39-4 3-Methylphenol

RX(13) RCT S 19857-34-2  
RGT Q 7446-08-4 SeO2  
PRO U 58980-14-6  
CAT 108-24-7 Ac2O

RX(60) OF 73 COMPOSED OF RX(9), RX(22), RX(11)  
RX(60) N + T ==> S



RX(9) RCT N 28565-98-2  
PRO J 58980-13-5  
CAT 108-24-7 Ac2O

RX(22) RCT J 58980-13-5, T 62-53-3  
PRO R 74772-50-2  
CAT 108-39-4 3-Methylphenol

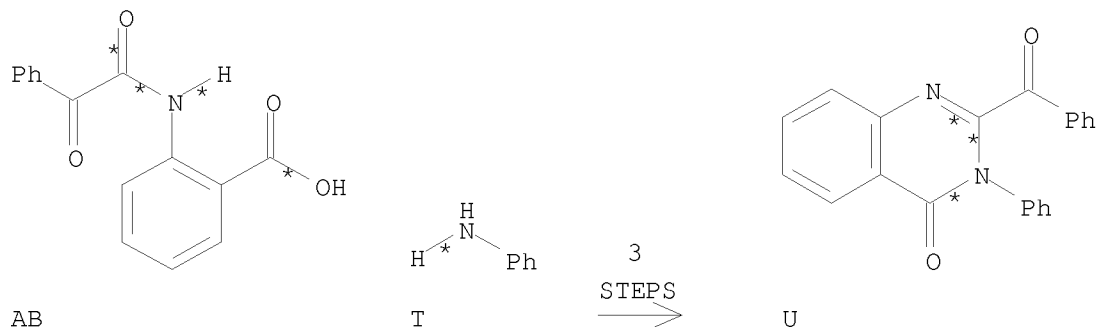
RX(11) RCT R 74772-50-2  
PRO S 19857-34-2  
CAT 108-39-4 3-Methylphenol



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RX(68) OF 73 COMPOSED OF RX(26), RX(23), RX(27)

RX(68) AB + T ==> U



RX(26) RCT AB 58980-12-4

PRO P 28565-99-3

CAT 108-24-7 Ac2O

RX(23) RCT P 28565-99-3, T 62-53-3

PRO AA 341545-11-7

CAT 108-39-4 3-Methylphenol

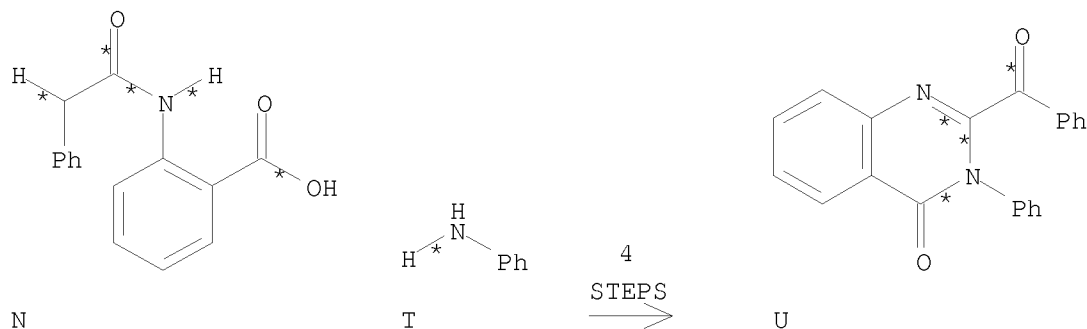
RX(27) RCT AA 341545-11-7

PRO U 58980-14-6

CAT 108-39-4 3-Methylphenol

RX(69) OF 73 COMPOSED OF RX(9), RX(10), RX(23), RX(27)

RX(69) N + T ==> U



RX(9) RCT N 28565-98-2

PRO J 58980-13-5

CAT 108-24-7 Ac2O

RX(10) RCT J 58980-13-5

RGT Q 7446-08-4 SeO2

PRO P 28565-99-3

CAT 108-24-7 Ac2O

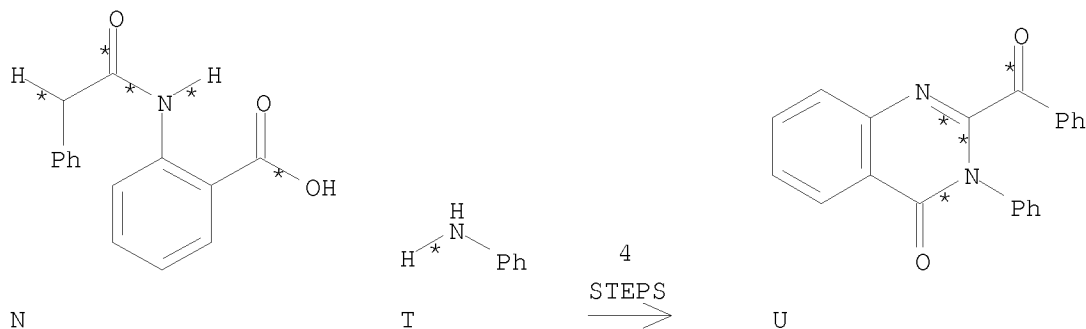
RX(23) RCT P 28565-99-3, T 62-53-3

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PRO AA 341545-11-7  
CAT 108-39-4 3-Methylphenol

RX(27) RCT AA 341545-11-7  
PRO U 58980-14-6  
CAT 108-39-4 3-Methylphenol

RX(71) OF 73 COMPOSED OF RX(9), RX(22), RX(11), RX(13)  
RX(71) N + T ==> U



RX(9) RCT N 28565-98-2  
PRO J 58980-13-5  
CAT 108-24-7 Ac2O

RX(22) RCT J 58980-13-5, T 62-53-3  
PRO R 74772-50-2  
CAT 108-39-4 3-Methylphenol

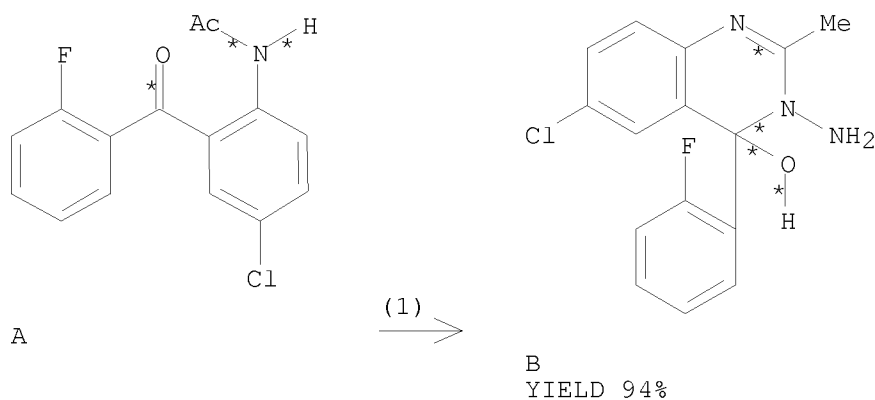
RX(11) RCT R 74772-50-2  
PRO S 19857-34-2  
CAT 108-39-4 3-Methylphenol

RX(13) RCT S 19857-34-2  
RGT Q 7446-08-4 SeO2  
PRO U 58980-14-6  
CAT 108-24-7 Ac2O

L3 ANSWER 250 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 83:193188 CASREACT  
TITLE: Quinazolines and 1,4-benzodiazepines. LXXI.  
Reactions of 2-(triazol-4-yl)benzophenones  
AUTHOR(S): Walser, Armin; Flynn, Thomas; Fryer, R. Ian  
CORPORATE SOURCE: Res. Div., Hoffmann-La Roche, Inc., Nutley, NJ, USA  
SOURCE: Journal of Heterocyclic Chemistry (1975), 12(4),  
717-24  
CODEN: JHTCAD; ISSN: 0022-152X  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI For diagram(s), see printed CA Issue.  
AB Some new triazolybenzophenones, e.g. I (R = H), were prepared by reaction

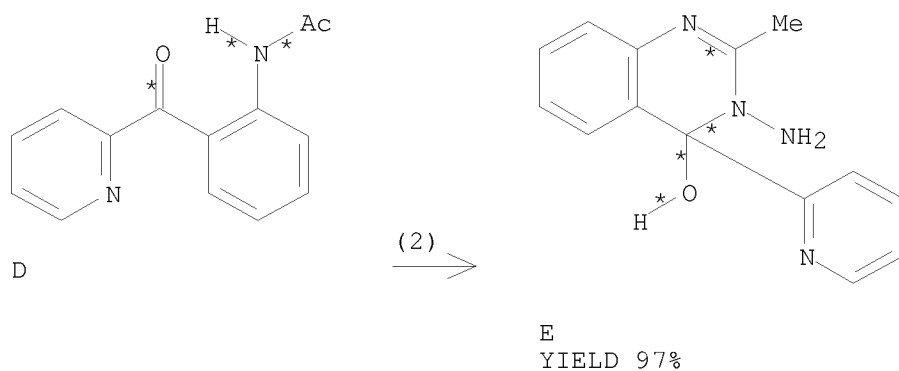
of the corresponding quinazolines, e.g. II, with  $\text{HCO}_2\text{H}$ . The triazolylbenzophenones were converted to triazolobenzodiazepines, e.g. III. The reaction of I ( $\text{R} = \text{CHO}$ ) with hydrazine yielded the triazoloquinolines IV and V. The cyclization of the benzophenones, e.g. I ( $\text{R} = \text{H}$ ), gave triazoloindoles, e.g. VI ( $\text{R} = \text{H}$ ), which were alkylated to derivs. with basic and acidic side chains. Quaternization of compound VI ( $\text{R} = \text{CH}_2\text{CO}_2\text{Et}$ ) with  $\text{BrCH}_2\text{CO}_2\text{Et}$  followed by treatment with hydroxide resulted in the formation of the triazinoindole V.

RX(1) OF 49      A    ==>   B...



RX(1)      RCT   A 57698-59-6  
              RGT   C 302-01-2  $\text{N}_2\text{H}_4$   
              PRO   B 57698-27-8

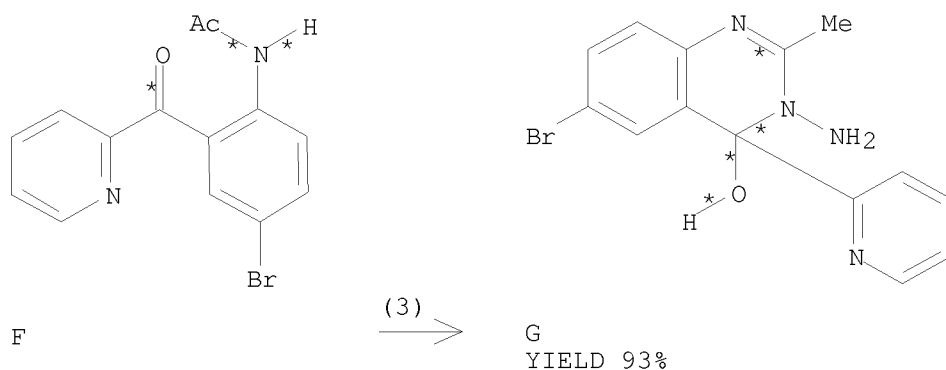
RX(2) OF 49      D    ==>   E...



RX(2)      RCT   D 1770-89-4  
              RGT   C 302-01-2  $\text{N}_2\text{H}_4$   
              PRO   E 57698-28-9

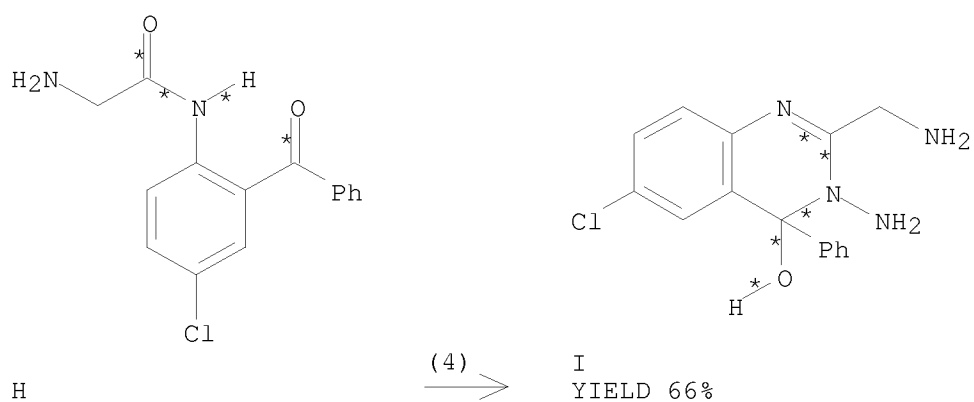
RX(3) OF 49      F    ==>   G...

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RX(3)      RCT    F 1770-90-7  
              RGT    C 302-01-2 N2H4  
              PRO    G 57698-29-0

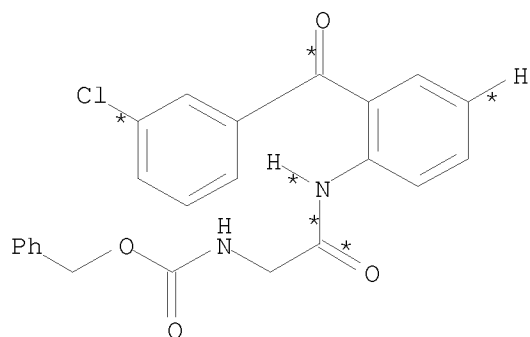
RX(4) OF 49      H ==> I



RX(4)      RCT    H 5504-71-2  
              RGT    C 302-01-2 N2H4  
              PRO    I 57698-31-4

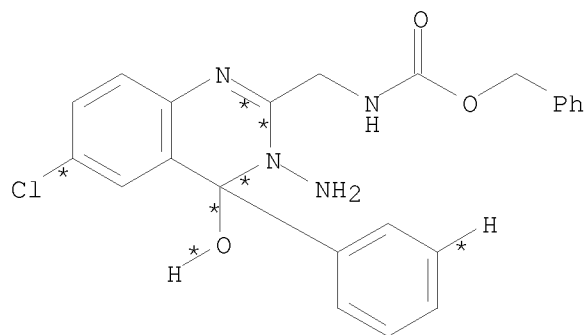
RX(5) OF 49      J ==> K...

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J

(5)  $\longrightarrow$

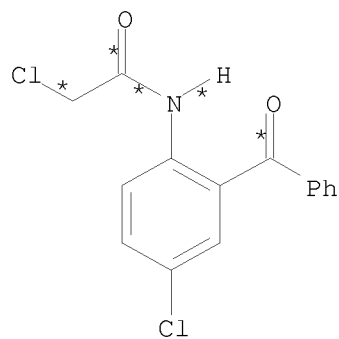


K

YIELD 67%

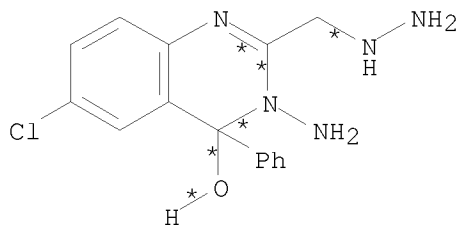
RX(5)      RCT   J 340171-33-7  
               RGT   C 302-01-2 N2H4  
               PRO   K 57698-32-5

RX(6) OF 49      L     $\implies$     M



L

(6)  $\longrightarrow$



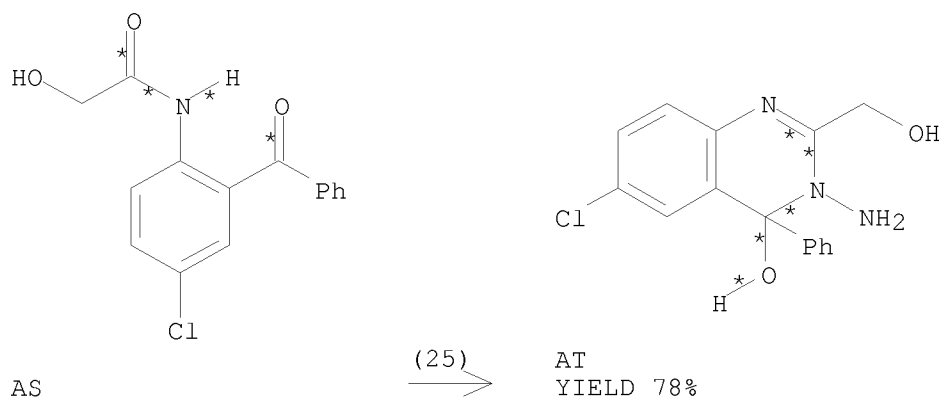
M

YIELD 78%

10/ 562,112

RX(6)        RCT    L 4016-85-7  
             RGT    C 302-01-2 N2H4  
             PRO    M 57698-33-6

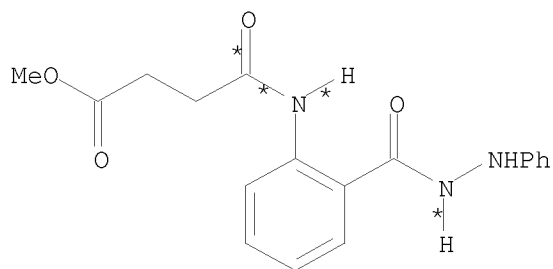
RX(25) OF 49        AS    ==>    AT...



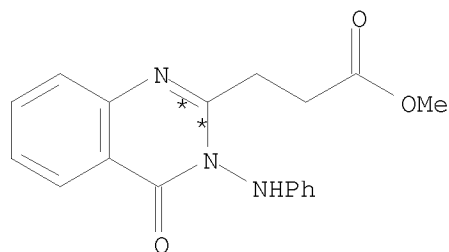
RX(25)        RCT    AS 5628-03-5  
             RGT    C 302-01-2 N2H4  
             PRO    AT 57698-30-3

L3    ANSWER 251 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER:        83:28178    CASREACT  
TITLE:                    4-Quinazolone series. VI. Synthesis and properties  
                            of 2-( $\beta$ -carbmethoxyethyl)-3-arylamino-substituted  
                            4-quinazolone  
AUTHOR(S):                Kozhevnikov, Yu. V.  
CORPORATE SOURCE:        Perm. Farm. Inst., Perm, USSR  
SOURCE:                    Izvestiya Vysshikh Uchebnykh Zavedenii, Khimiya i  
                            Khimicheskaya Tekhnologiya (1975), 18(2), 235-7  
                            CODEN: IVUKAR; ISSN: 0579-2991  
DOCUMENT TYPE:            Journal  
LANGUAGE:                  Russian  
GI    For diagram(s), see printed CA Issue.  
AB    4-Quinazolinones (I; R = H, o-, m-, p-Me, o-, m-, p-Cl, o-, m-, p-Br,  
         4-bromo-2-methyl) were prepared in 30-88% yields by reaction of  
         benzoxazinepropionate (II) with RC6H4NHNH2 in PhMe containing PCl3.

RX(1) OF 14        ...A    ==>    B



A



B

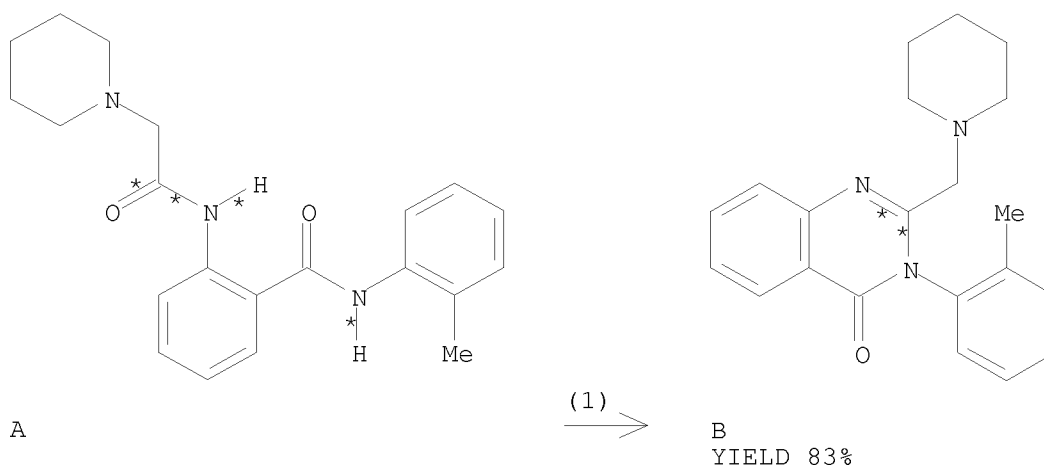
YIELD 31%

RX(1)      RCT    A 56056-26-9  
              RGT    C 7719-12-2 PC13  
              PRO    B 56056-14-5

L3    ANSWER 252 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER:      69:96650    CASREACT  
 TITLE:                    2-Dialkylaminomethyl- and  
                               2-[ $\beta$ -(dialkylamino)ethyl]-3-aryl-4-oxo-3,4-  
                               dihydroquinazoline  
 AUTHOR(S):                Pesson, Marcel; Richer, Denise  
 CORPORATE SOURCE:      Lab. Roger Bellon, Neuilly-sur-Seine, Fr.  
 SOURCE:                    Comptes Rendus des Seances de l'Academie des Sciences,  
                               Serie C: Sciences Chimiques (1968), 266(26), 1787-90  
                               CODEN: CHDCAQ; ISSN: 0567-6541  
 DOCUMENT TYPE:          Journal  
 LANGUAGE:                French  
 GI    For diagram(s), see printed CA Issue.  
 AB    I, where n is 1 or 2 and R is piperidino, are prepared Thus,  
       o-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CONHC<sub>6</sub>H<sub>4</sub>Me-o is treated with ClCH<sub>2</sub>COCl in a NaOAcHOAc mixture to  
       give 69% o-ClCH<sub>2</sub>CONHC<sub>6</sub>H<sub>4</sub>CONHC<sub>6</sub>H<sub>4</sub>Me-o (II), m. 180°. Similarly  
       prepared are o-ClCH<sub>2</sub>CONHC<sub>6</sub>H<sub>4</sub>CONHPh, m. 190°, and  
       o-ClCH<sub>2</sub>CH<sub>2</sub>CONHC<sub>6</sub>H<sub>4</sub>CONHC<sub>6</sub>H<sub>4</sub>Me-o, m. 173°. A mixture of II,  
       piperidine, and C<sub>6</sub>H<sub>6</sub> is refluxed to give o-(piperidinoacetamido)benzoic  
       acid o-toluidide (III), m. 163°. Similarly prepared are

o-(piperidinoacetamido)benzanilide, m. 176°, and o-(β-piperidinopropionamido)benzoic acid o-toluidide, m. 114-15°. A mixture of III and HOAc is refluxed 6 hrs. to give 83% 2-(piperidinomethyl)-3-(o-tolyl)-4-oxo-3,4-dihydroquinazoline (IV), m. 88-9°. Similarly prepared are I (n = 1, R = piperidino, Ar = Ph), m. 128°, and I (n = 2, R = piperidino, Ar = o-tolyl) (V) (prepared in anisole), 121°. Uv and ir data for IV and V and N.M.R. data for IV are given. A mixture of III and Ac<sub>2</sub>O is heated to give o-AcNHC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H (m. 192°) and N,N-pentamethyleneglycine o-toluidide (m. 96-8°). A mixture of II in HOAc is refluxed to give I (n = 1, R = Cl, Ar = o-tolyl) (VI), m. 108-10°, which is hydrogenated (5% Pd/C) to give I (n = 1, R = H, Ar = o-tolyl), m. 115°. A mixture of VI, piperidine, and C<sub>6</sub>H<sub>6</sub> is refluxed to give IV, m. 88-90°.

RX(1) OF 1 A ==&gt; B



RX(1) RCT A 19806-75-8  
 RGT C 64-19-7 AcOH  
 PRO B 19806-76-9  
 NTE Classification: Condensation; Heterocycle formation;  
 Cyclisation; # Conditions: AcOH heat 6h

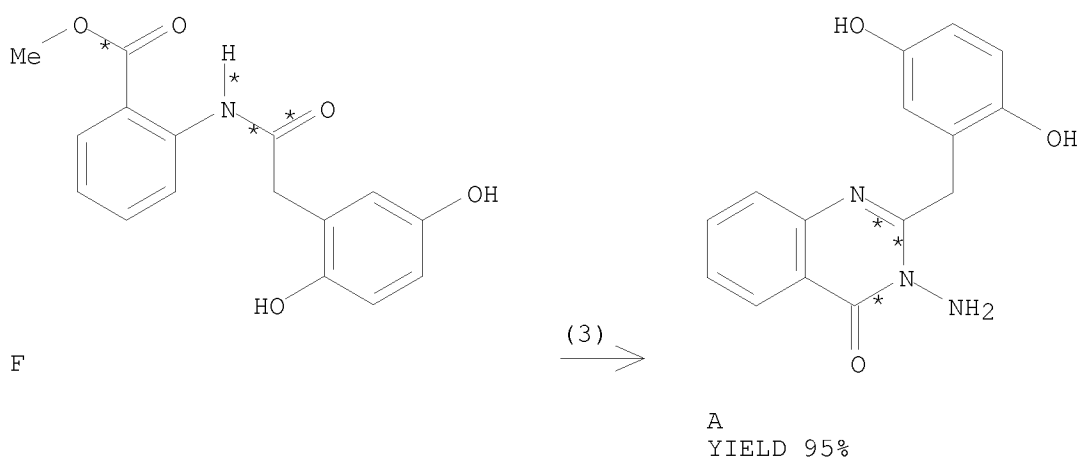
L3 ANSWER 253 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 66:18698 CASREACT  
 TITLE: Preparation and properties of some substituted  
 quinazolino[3,2-b]cinnolines  
 AUTHOR(S): Kort, M. J.; Lamchen, Max  
 CORPORATE SOURCE: Univ. Cape Town, Cape Town, S. Afr.  
 SOURCE: Journal of the Chemical Society [Section] C: Organic  
 (1966), (23), 2190-6  
 CODEN: JSOOAX; ISSN: 0022-4952  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI For diagram(s), see printed CA Issue.  
 AB The prepn. of the substituted quinol



3-amino-2-(2,5-dihydroxybenzyl)quinazolin-4(3H)-one (I) and some of its derivs. are described. When this quinol is oxidized with an acidic ferric chloride solution or with an aqueous sodium hydroxide solution a quinone was formed,

but it spontaneously ring-closed to give quinazolino[3,2-b]cinnoline-2,7(13H)-dione (II), which was isolated as the hydrochloride. When the oxidation of the quinol was carried out with an acidic hydrogen peroxide solution the ring-closed product also formed as an intermediate, which was immediately converted into 1,3,4-trichloroquinazolino[3,2-b]cinnoline-2,7(13H)-dione, and only this dione was then obtained.

RX(3) OF 6 ...F ==> A...



RX(3) RCT F 13162-86-2  
 RGT G 302-01-2 N2H4  
 PRO A 13162-88-4  
 SOL 7732-18-5 Water, 64-17-5 EtOH  
 NTE Classification: Annellation; Condensation; Hydrazination;  
 Heterocycle formation; # Conditions: N2H4 H2O EtOH; Rf 3h

L3 ANSWER 254 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 55:13443 CASREACT  
 TITLE: 2,3-Disubstituted 3H-4-quinazolones and  
 3H-4-thioquinazolones  
 AUTHOR(S): Jackman, G. B.; Petrow, V.; Stephenson, O.  
 SOURCE: Journal of Pharmacy and Pharmacology (1960), 12,  
 529-38  
 CODEN: JPPMAB; ISSN: 0022-3573  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB Typical procedures in the synthesis of some  
 2-alkyl-3-aryl-3H-4-quinazolones and conversion to thio derivs. follow. A  
 solution of 8 ml. PCl3 in 50 ml. PhMe was added to a stirred mixture of 34.4 g.  
 p-bromoaniline (I) and acetylanthranilic acid (II) at room temperature, the  
 resulting paste was refluxed 2 hrs., cooled, 15% Na2CO3 solution added, and

the PhMe steam-distilled to give 27 g.

3-p-bromophenyl-2-methyl-3H-4-quinazolone (III), which was crystallized from 95% EtOH; HCl salt (IV) m. approx. 260° (decomposition) (95% EtOH).

Addition of 11.4 g. dicyclohexylcarbodiimide in 50 ml. tetrahydrofuran (THF) to 8.9 g. I and 9 g. II in 100 ml. THF and, after 5 hrs. at room temperature, addition of 1.5 ml. AcOH, precipitated dicyclohexylurea, which was filtered off after 2 hrs. Evaporation of the filtrate to dryness in vacuo, dissoln. of the residue in 150 ml. EtOAc and shaking with 2N HCl precipitated 9 g. IV; and washing the filtered EtOAc solution with 1N Na<sub>2</sub>CO<sub>3</sub> and H<sub>2</sub>O, then concentrating

to 50

ml. gave 1.5 g. 2-acetamido-4'-bromobenzanilide, m. 215-16°.

PhSO<sub>2</sub>Cl (17.8 g.) was added to 17.9 g. II in 30 ml. C<sub>5</sub>H<sub>5</sub>N then 16.2 g.

2,4-dichloroaniline was added portionwise, the mixture heated 2 hrs. over steam, cooled, and diluted with H<sub>2</sub>O to give

3-(2,4-dichlorophenyl)-2-methyl-3H-quinazolone as a gum which solidified on trituration with EtOH and yielded 9.6 g. needles, m. 151-2°

(EtOAc-petr. ether); HCl salt m. 242-50° (MeOH). A mixture of II and

2,4-dichloroaniline in C<sub>5</sub>H<sub>5</sub>N with PCl<sub>3</sub> added dropwise gave the above product, separated as the HCl salt, m. 240-50°. Prepared as

intermediates were (m.p. given): 4-bromo-2,3-dimethylacetanilide,

158-60° (long needles, aqueous-EtOH) [HCl salt, m. 268°

(decomposition), with NaOH and steam distillation gave

4-bromo-2,3-dimethylaniline,

m. 32-4° (plates, petr. ether)];

4-bromo-2,3-dimethyl-6-nitroacetanilide, 207-9° (pale yellow

needles, 95% EtOH); 4-bromo-2,3-dimethyl-6-nitroaniline, 147-9°

(flat golden-brown needles, 50% EtOH);

5-bromo-3,4-dimethyl-o-phenylenediamine, 85-7° (petr. ether). The

following 2-alkyl-3-aryl-3H-4-quinazolones were prepared (alkyl and aryl substituents, resp., base or HCl salt, indicated by B or H, resp., and

m.p. given; all the HCl salts melted with decomposition over a range of several

degrees): Me, p-anisyl, H 240°; Me, o-phenetyl, B 115-16°, H

215°; Me, m-phenetyl, B 130-2°, H 225°; Me,

p-phenetyl, H 240°; Me, 3,4,5-trimethoxyphenyl, B 150-2°, H

250°; Me, 2,3-xylyl, B 172-3°, H 240°; Me, 2,4-xylyl,

B 100-2°, H 240°; Me, 2,5-xylyl, B 125-7°; Me,

2,6-xylyl, H 215°; Me, 3,4-xylyl, B 134-6°; Me, p-FC<sub>6</sub>H<sub>4</sub>, B

133-4°, H 280°; Me, o-ClC<sub>6</sub>H<sub>4</sub>, B 130-2°; Et, o-ClC<sub>6</sub>H<sub>4</sub>,

B 124-6°; Me, m-ClC<sub>6</sub>H<sub>4</sub>, B 133-5°; Me, o-BrC<sub>6</sub>H<sub>4</sub>, B

147-8°, H 220°; Me, m-BrC<sub>6</sub>H<sub>4</sub>, B 134-6°, H

260°; Me, p-BrC<sub>6</sub>H<sub>4</sub>, B 170-2°, H 260°; Et, p-BrC<sub>6</sub>H<sub>4</sub>, B

170-2°; Pr, p-BrC<sub>6</sub>H<sub>4</sub>, B 139-41°; Me, p-IC<sub>6</sub>H<sub>4</sub>, B

178-80°, H 265°; Me, 2,4-ClC<sub>6</sub>H<sub>3</sub>, B 151-2°, H

250°; Me, 2,5-Cl<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, B 161-3°, H 244°; Me,

4-bromo-2,3-xylyl, B 168-70°. Thioquinazolone derivs. were prepared

by refluxing the quinazolone with P<sub>2</sub>S<sub>5</sub> in xylene, cooling, adding NaOH and distilling with steam. 2-Alkyl-3-aryl-3H-4-thioquinazolones prepared were

(alkyl, aryl, base or HCl salt, and m.p. given, resp.): Me, o-tolyl, B

121-3°, H 228-30°; Me, p-FC<sub>6</sub>H<sub>4</sub>, B 128-30°; Me,

p-ClC<sub>6</sub>H<sub>4</sub>, B 183-5°; Me, o-BrC<sub>6</sub>H<sub>4</sub>, B 174-6°; Me, p-BrC<sub>6</sub>H<sub>4</sub>, B

190-2°; Et, p-BrC<sub>6</sub>H<sub>4</sub>, B 168-70°.

N-Alkyl-2-benzamidobenzamides prepared were (alkyl at -CONHR, aryl at

-NHCOAr, and m.p., resp.): H, p-BrC<sub>6</sub>H<sub>4</sub>, 224-6°; Me, o-tolyl,

167-70°; Me, p-ClC<sub>6</sub>H<sub>4</sub>, 162-4° and 190-2°; Me,

o-BrC<sub>6</sub>H<sub>4</sub>, 170-2°; Me, p-BrC<sub>6</sub>H<sub>4</sub>, 165° and 197-9°; Et,

Ph, 158-60°; Et, p-BrC<sub>6</sub>H<sub>4</sub>, 174-6°; Bu, Ph, 125-7°.

3-Methyl-2-o-tolyl-3H-4-quinazolone was prepared by refluxing 26.7 g.

N-methyl-2-(o-methylbenzamido)benzamide with 300 ml. 5% NaOH containing 50 ml.

EtOH, and also from 4 g. 2-o-tolyl-3H-4-quinazolone in 80 ml. 1N NaOH and

Me<sub>2</sub>SO<sub>4</sub> (dropwise). The products (56% and 50%, resp.) were purified by

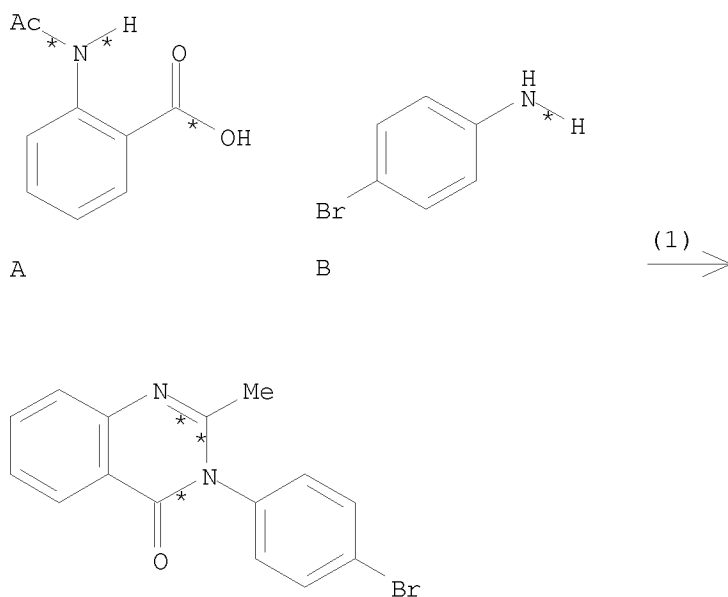
crystallization from petr. ether and aqueous EtOH. The HCl salt crystallized from EtOH.

The 3-alkyl-2-aryl-3H-4-quinazolones prepared were (alkyl, aryl, base or HCl salt, and m.p., resp., given): Me, Ph, B 136-8°, H 208° (decomposition); Et, Ph, B 130-2°, H 205° (decomposition); Bu, Ph, B 116-18°; 2,3-dihydroxypropyl, Ph, B 179-81°; Me, o-tolyl, B 107-9°, H 205° (decomposition); Me, p-ClC<sub>6</sub>H<sub>4</sub>, B 170-2°; Me, o-BrC<sub>6</sub>H<sub>4</sub>, B 154-6°; H, p-BrC<sub>6</sub>H<sub>4</sub>, B 313-5°; Me, p-BrC<sub>6</sub>H<sub>4</sub>, B 170-2°; Et, p-BrC<sub>6</sub>H<sub>4</sub>, 122-4°, 138-40°.

2-p-Bromophenyl-3-methyl-3H-4-quinazolone (44.1 g.) in 400 ml. xylene was refluxed 2 hrs. with 37.4 g. P<sub>2</sub>S<sub>5</sub>, 275 ml. 10% NaOH was added cautiously to the cooled mixture, and the xylene steam-distilled to give 42 g.

2-p-bromophenyl-3-methyl-3H-4-thioquinazolone, m. 167-9°, yellow hair-like crystals from 2 l. EtOH.

RX(1) OF 1      A + B ==> C



C  
YIELD 45%

RX(1)      RCT    A 89-52-1, B 106-40-1  
              PRO    C 1788-95-0  
              SOL    108-88-3 PhMe  
              NTE    Classification: Heterocycle formation; C-Amination;  
                      Condensation; # Conditions: PCl<sub>3</sub> toluene; 20 deg; Rf 2h

L3    ANSWER 255 OF 258    CASREACT    COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER:        52:50665    CASREACT  
 TITLE:                      Research in the 2-methyl-3-aryl-4-quinazolone series  
 AUTHOR(S):                Serventi, Giorgio; Marchesi, Renato  
 CORPORATE SOURCE:        Univ. Parma, Italy

SOURCE: Bollettino Scientifico della Facolta di Chimica  
Industriale di Bologna (1957), 15, 117-20  
CODEN: BSFCAY; ISSN: 0366-3205

DOCUMENT TYPE: Journal

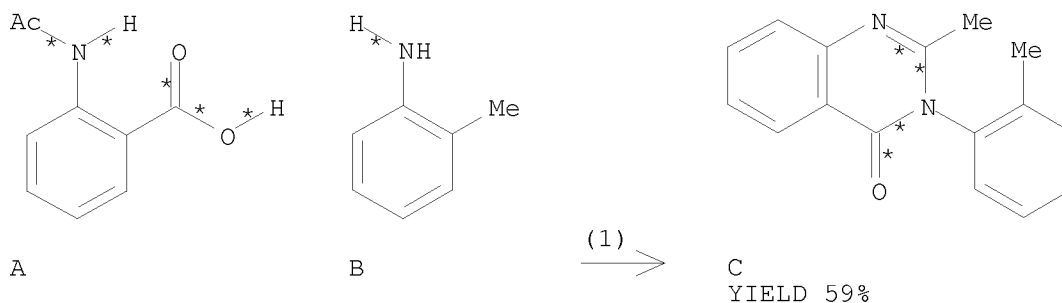
LANGUAGE: Unavailable

AB This series was studied for its promise of yielding antimalarial and analgesic agents.  $\text{PCl}_3$  (0.033 mole) in 20 cc. PhMe added dropwise to 0.1 mole acetylanthranilic acid and 0.1 mole arylamine in 200 cc. PhMe, the mixture refluxed 2 hrs. and made alkaline with aqueous  $\text{Na}_2\text{CO}_3$  (10%), and the solid

recrystd. several times gave 2-methyl-3-aryl-4-quinazolones (3-aryl group, m.p., and % yield given): Ph,  $146-7^\circ$ , 86; o-tolyl (o-I),  $120^\circ$ , 59; m-I,  $129^\circ$ , 51; p-I,  $149-50^\circ$ , 68; o-chlorophenyl (o-II),  $120^\circ$ , 43; m-II,  $130^\circ$ , 63.19; p-II,  $157^\circ$ , 80; o-anisyl (o-III),  $132^\circ$ , 55.3; m-III,  $152^\circ$ , 72; p-III,  $170^\circ$ , 70; o-carbomethoxyphenyl (o-IV),  $120^\circ$ , 53.2; m-IV,  $132^\circ$ , 48; p-IV,  $198^\circ$ , 65.3.

2-Methyl-3-(o-carboxyphenyl)-4-quinazolone was prepared by treating 0.1 mole I with 0.15 mole NaOH in 50 cc. EtOH (50%), refluxing 4 hrs., acidifying, and crystallizing from AcOH, m.  $246-7^\circ$ , yield 33%; the m-isomer m.  $276^\circ$ , yield 42.5%; p-isomer, m.  $281^\circ$ , yield 39.5%. A table of ultraviolet spectral data at three wavelengths is also given.

RX(1) OF 1      A + B ==> C



RX(1)      RCT    A 89-52-1, B 95-53-4  
             PRO    C 72-44-6  
             SOL    108-88-3 PhMe  
             NTE    Classification: Annellation; Heterocycle formation; C-Amination;  
                     Condensation; # Conditions:  $\text{PCl}_3$  toluene; Rf 2h; # Comments:  
                     Also C.A., 9147 (1958).

L3      ANSWER 256 OF 258      CASREACT    COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER:      51:85734    CASREACT

TITLE:      Preparation of quinazoline derivatives through  
                 ring-closure of aromatic o-cyano(acylamino) compounds  
                 in alkaline alcoholic or phenolic medium. I.  
                 4-RO-substituted quinazolines

AUTHOR(S):      Breukink, K. W.; Krol, L. H.; Verkade, P. E.; Wepster,

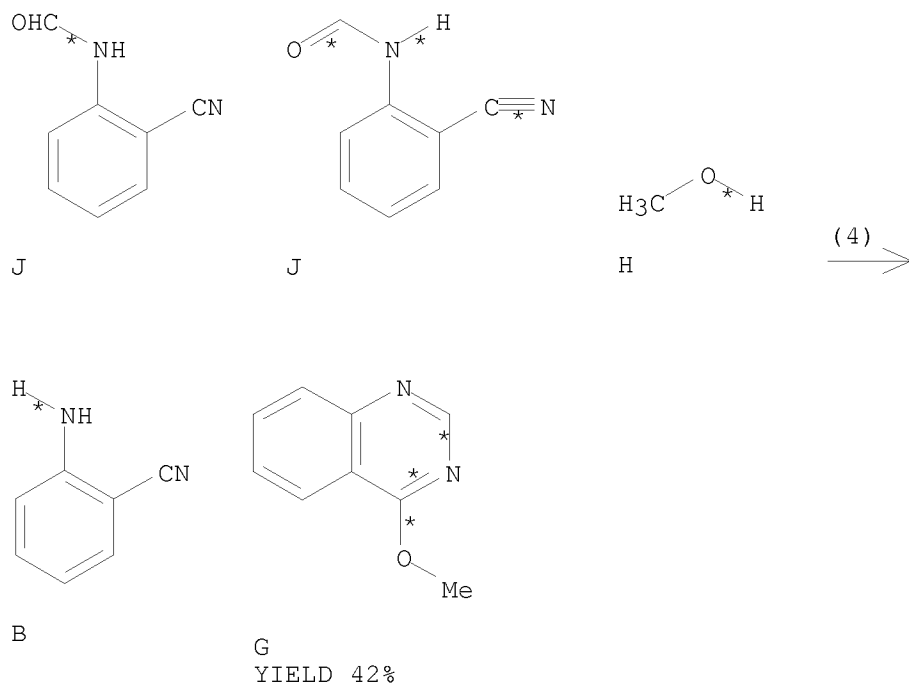
B. M.  
 CORPORATE SOURCE: Tech. Univ., Delft, Neth.  
 SOURCE: Recueil des Travaux Chimiques des Pays-Bas et de la  
 Belgique (1957), 76, 401-14  
 CODEN: RTCPB4; ISSN: 0370-7539

DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB On boiling aromatic o-cyano(acylamino) compds. in alkaline alc. or phenolic solution, 4-RO substituted quinazolines are formed. The diazonium salt from the diazotization of o-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> (cf. Fieser and Thompson, C.A. 33, 21211) treated according to Bogert and Hand [J. Am. Chemical Society 24, 1035(1902)] yielded pure o-NCC<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>, m. 109-10°, reduced with SnCl<sub>2</sub> and concentrated HCl, and the product purified by distillation in vacuo to give-82% pure o-NCC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> (I), b<sub>18</sub> 138-9°; picrate, m. 108-9° I (6.10 g.) in 75 ml. dry Et<sub>2</sub>O and 8.5 ml. freshly prepared AcOCHO (cf. Clemons and Swan, C.A. 40, 5811) filtered after 24 hrs. and the crystalline product (7.11 g.) recrystd. from 1:1 C<sub>6</sub>H<sub>6</sub>-petr. ether gave 6.92 g. pure o-NCC<sub>6</sub>H<sub>4</sub>NHCHO (II), m. 130.5-1.5°. II (5.00 g.) refluxed with 75 ml. 0.05N NaOMe in absolute MeOH with addition of 5, 5, and 10 ml. 0.5N NaOMe in MeOH after 2, 3, and 3.5 hrs., the alkaline solution distilled in vacuo after 4 hrs., the residue extracted with Et<sub>2</sub>O, the washed and dried extract evaporated, and the residue distilled in vacuo gave 4.83 g. strongly hygroscopic oil, treated with 50 ml. petr. ether 24 hrs. at room temperature to give 1.69 g. I, m. 48-9°. The petr. ether mother liquor filtered and evaporated, the residue taken up in 50 ml. MeOH, treated with 4 g. picric acid in 25 ml. MeOH, and filtered immediately, the precipitate washed with MeOH, dried, and crystd, from PhMe gave 5.31 g. picrate, m. 175.5-6.5°, decomposed with aqueous LiOH and extracted with Et<sub>2</sub>O to give 4-methoxyquinazoline (III), m. 35-6°, b<sub>11</sub> 127-8°, strongly hygroscopic. Conversion of the known 4-hydroxyquinazoline (IIIa) according to Endicott, et al. (C.A. 40, 57482), gave 4-chloroquinazoline (IV), m. 97-8°. On completion of the exothermic reaction between 10 g. IV and 100 ml. N NaOMe in MeOH, the mixture was boiled 15 min., the MeOH evaporated in vacuo, and the residue treated with Et<sub>2</sub>O and H<sub>2</sub>O, the Et<sub>2</sub>O extract dried and evaporated, and the residue fractionated in vacuo to give 7.3 g. III, converted to IIIa by boiling in dilute HCl. I (6.00 g.) in 100 ml. dry Et<sub>2</sub>O kept 24 hrs. at room temperature with 15 ml. Ac<sub>2</sub>O and filtered gave 7.91 g. o-NCC<sub>6</sub>H<sub>4</sub>NHAc (V), m. 133-4° (from Et<sub>2</sub>O). V (5.00 g.) refluxed in 100 ml. 0.05N NaOMe in MeOH and treated after 2 and 4 hrs. with 5 and 10 ml. 0.5N NaOMe in MeOH, and the solution worked up after 5 hrs. refluxing gave 5.20 g. colorless oil, treated with 40 ml. petr. ether to give 0.30 g. I on filtration after keeping 24 hrs. at room temperature. The petr. ether mother liquor distilled in vacuo, the residue taken up in 50 ml. MeOH, the solution diluted with H<sub>2</sub>O, cooled to 0°, kept 1 week with further dilution with H<sub>2</sub>O, and filtered gave 6.05 g. trihydrate, m. 36-7°, dehydrated at 65°/20 mm. to 4-methoxy-2-methylquinazoline, m. 34-5°; picrate, m. 170.0-1.5°. Similarly, refluxing V with NaOEt in EtOH and working up gave 12% I and 82% monohydrate, m. 39.5-40.0°, dehydrated to 4-ethoxy-2-methylquinoline; picrate, m. 178.0-9.5°. V (5.00 g.) heated 20 hrs. at 120° with 0.35 g. Na in 50 ml. dry PhCH<sub>2</sub>OH, the alc. evaporated in vacuo, the residue suspended in 250 ml. 20% EtOH and filtered, and the crude precipitate crystallized from petr. ether gave 5.47 g. 4-benzyloxy-2-methylquinazoline, m. 65.5-6.0°; picrate, m.

147.5-8.5°. Similarly, heating 2.50 g. V 20 hrs. with 0.20 g. Na in 25 g. dry pure PhOH at 125°, the PhOH distilled in vacuo, and the residue suspended in 100 ml. 2N NaOH filtered, the precipitate taken up in Et2O, the washed and dried extract evaporated, the residue taken up in 40 ml. MeOH, treated with C, and filtered, the filtrate diluted with 30 ml. H2O and heated, and the solution cooled to 0° and filtered gave 3.52 g. monohydrate, m. 71-83°, dehydrated over P2O5 in vacuo to 4-phenoxy-2-methylquinazoline, m. 71.0-1.5°. The four 4-RO-2-methylquinazolines gave quant. yields of IIIa on boiling with dilute HCl. I (4.00 g.) and 5.8 g. BzCl in 100 ml. dry Et2O refluxed 2 hrs. with 4.8 g. anhydrous K2CO3, the Et2O evaporated in vacuo, the residue extracted with H2O and filtered, and the washed and dried precipitate recrystd. from MeOH gave 5.98 g. o-NCC6H4NHPh (VI), m. 159-60°. VI (5.00 g.) refluxed 6 hrs. with 90 ml. 0.1N NaOMe in MeOH, the solvent distilled in vacuo, and Et2O added to the residue, the washed and dried extract evaporated, and the residue distilled in vacuo gave 0.68 g. I and 3.60 g. fraction, b3 189-91°, recrystd. from dilute MeOH to give 3.55 g. 4-methoxy-2-phenylquinazoline, m. 65.5-6.0° (picrate, m. 174.0-5.5°), converted by boiling dilute HCl to 4-hydroxy-2-phenylquinazoline, m. 240-1°. Iodine (100 g.), 50.0 g. p-ClC6H4NH2, 50 g. CaCO3, 175 ml. Et2O, and 175 ml. H2O refluxed 48 hrs. and worked up according to Dains, et al. (C.A. 12, 1646), gave 61.5 g. 4,2-ClIC6H3NH2 (VII), m. 40.5-1.5°. The preferential replacement of iodine in VII by a CN group according to Brit. 488,642 (C.A. 33, 4011) gave 4,2-Cl(NC)C6H3NH2 (VIII), m. 95.0-5.5° (from 1:1 petr. ether-C6H6). VIII boiled 30 min. with 2N NaOH until evolution of NH3 ceased, the cold solution neutralized with HCl and saturated NaOAc solution and filtered, and the precipitate crystallized from H2O in the presence of C gave authentic 5-chloroanthranilic acid, m. 208.5-10.0°, proving the constitution of VIII and VII. VIII (5.00 g.) heated 2 hrs. at 50° in 10 ml. Ac2O, the mixture poured into 50 ml. H2O and filtered and the dried precipitate crystallized from 2:1 C6H6-petr. ether gave 6.05 g. 4,2-Cl(NC)C6H3NHAc (IX), m. 149.5-50.5°. Conversion of IX with no perceptible deacetylation or consumption of the alkaline catalyst rapidly gave 6-chloro-4-methoxy-2-methylquinazoline, m. 79-80° (from petr. ether), b12 155-6° (picrate, m. 168.0-9.5°), and 6-chloro-4-ethoxy-2-methylquinazoline, m. 98.5-9.5°, b13 160-1° (picrate, m. 188-9°). CuCN (3.5 g.) and 3.3 ml. dry pyridine treated with 25 g. dry PhNO2 and 9.60 g. 2-bromo- $\alpha$ -acetonaphthalide (cf. Hodgson and Hathway, C.A. 38, 20304), stirred 2 hrs. at 180-90°, the cooled mixture diluted with H2O, steam-distilled, and filtered, the washed precipitate dried and extracted several times with 5 ml. portions of EtOH, and the combined alc. exts. treated with C, cooled, and filtered gave 5.92 g. 2-cyano- $\alpha$ -acetonaphthalide (X), m. 219.5-20.5°. X (2.50 g.) refluxed 30 hrs. with 75 ml. 0.1N NaOMe in absolute MeOH, the alc. evaporated in vacuo, H2O added to the residue, the mixture filtered, and the washed and dried precipitate crystallized from MeOH gave 2.14 g. 4-methoxy-2-methylbenzo[h]quinazoline, m. 119-20°.

RX(4) OF 5      2 J + H ==> B + G

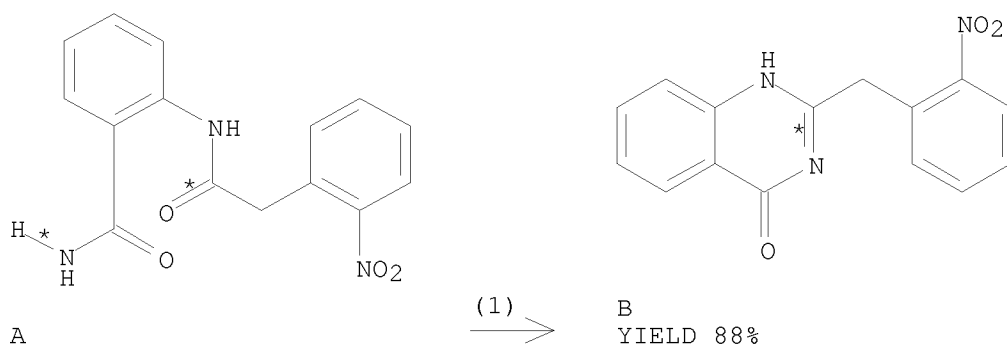


RX(4) RCT J 53902-59-3, H 67-56-1  
 PRO B 1885-29-6, G 16347-95-8  
 SOL 67-56-1 MeOH  
 NTE Classification: Deformylation; Heterocycle formation;  
 Alkoxylation; # Conditions: MeOH; boil Rf 4h; # Comments: 40%  
 yield of ring closure product as picrate; NaOMe used

L3 ANSWER 257 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 42:29858 CASREACT  
 TITLE: Quinazolines. V. The synthesis of 2- and  
 3-(o-aminobenzyl)-4-quinazolones  
 AUTHOR(S): Tomisek, A.; Christensen, Bert E.  
 CORPORATE SOURCE: Oregon State Coll., Corvallis  
 SOURCE: Journal of the American Chemical Society (1948), 70,  
 1701-2  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB cf. C.A. 42, 3413b. o-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>COC<sub>1</sub> (I) (from 5 g. of acid) and 4  
 mL. o-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Me in C<sub>6</sub>H<sub>6</sub>, gradually treated with 40 mL. 25% KOH,  
 give 69% Me N-(o-nitrophenylacetyl)anthranilate (II), m.  
 133.5-4° (m.ps. corrected); heated 8 h. at 180° with absolute alc.  
 NH<sub>3</sub>, it gives a good yield of o-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CONH<sub>2</sub>; the Ac derivative of  
 II (not isolated), heated with 14% NH<sub>4</sub>OH containing a little 10% KOH (1 h. on  
 the steam bath), gives 2-methyl-4(3H)-quinazolinone, indicating that  
 transacylation to o-MeO<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>NHAc had preceded the cyclization. I  
 (from 5 g. acid) and 7.6 g. o-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CONH<sub>2</sub> in dioxane give 73%  
 N-(o-nitrophenyl-acetyl)anthranilamide (III), m. 172-3°;

3.46 g. III, 12 mL. C<sub>5</sub>H<sub>5</sub>N, 12 mL. H<sub>2</sub>O, and 1 mL. 10% NaOH, kept 1 day at room temperature, yield 88% 2-*o*-nitrobenzyl-4(3H)-quinazolone (IV), m. 254.5° (decomposition). I (from 5 g. acid) and 20 g. *o*-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H in dioxane give 82% N-(*o*-nitrophenyl-acetyl)anthranilic acid (V), m. 224-5° (slow decomposition); 5 g. V and 20 mL. Ac<sub>2</sub>O, refluxed 30 min., give 4.4 g. 2-*o*-nitrobenzyl-4-keto-3,1,4-benzoxazine (VI), m. 165-6°; 5 g. VI in 25 mL. 50% C<sub>5</sub>H<sub>5</sub>N, saturated with NH<sub>3</sub>, allowed to stand 6 h., 1 mL. 10% NaOH added, and the mixture allowed to stand an addnl. 24 h., gives 72% IV. Treatment of 5 g. IV in 300 mL. dilute NaOH with 33 g. FeSO<sub>4</sub>·9H<sub>2</sub>O in 100 mL. H<sub>2</sub>O 7 h. at 80° gives 80% 2-(*o*-aminobenzyl)-4(3H)-quinazolone, m. above 250° (decomposition); Ac derivative m. 258°. 4-Hydroxy-4(3H)-quinazolone (13 g.), 10 g. *o*-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>Cl, 5.9 g. 85% KOH, and 200 mL. EtOH, refluxed 6 h., the EtOH removed, and the residue refluxed 15 min. with dilute HCl and C<sub>6</sub>H<sub>6</sub>, give 3 g. 3-*o*-nitrobenzyl-4(3H)-quinazolone, m. 169-70°; reduction with SnCl<sub>2</sub> and HCl in AcOH gives 64% 3-(*o*-aminobenzyl)-4-(3H)-quinazolone, m. 178°.

RX(1) OF 1 A ==&gt; B



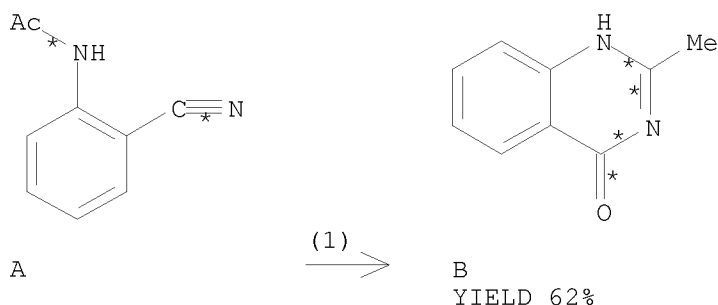
RX(1) RCT A 349135-30-4  
 PRO B 7494-72-6  
 SOL 7732-18-5 Water, 110-86-1 Pyridine  
 NTE Classification: Heterocycle formation; Cyclisation;  
 Condensation; Isomerisation; # Conditions: NaOH; H<sub>2</sub>O pyridine;  
 20 deg 1day

L3 ANSWER 258 OF 258 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 0:406 CASREACT  
 TITLE: The synthesis of alkylketodihydroquinazolines from anthranilic nitrile  
 AUTHOR(S): Bogert, Marston Taylor; Hand, William Flowers  
 CORPORATE SOURCE: Havemeyer Laboratories, Columbia University, USA  
 SOURCE: Journal of the American Chemical Society (1902), 24, 1031-1050  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Bogert and Gotthelf have already shown that ketodihydroquinazolines may be



prepared by heating together in sealed tubes anthranilic acid, or its acyl derivatives, with a nitrile, and the reactions there suggested in explanation of this synthesis, taking the case where an acylanthranilic acid was the starting-point. It will be seen upon examining the structure of the hypothetical intermediate product, the secondary amide, that the -CO-NH-CO- group being symmetrical should be formed equally well from RCN + R'.COOH as from R'CN + R.COOH; in other words, as the condensation takes place solely between the CN and COOH it is immaterial which radical carries the CN and which the COOH. This same secondary amide should therefore result when acetylanthranilic nitrile is heated with acetic acid.

RX(1) OF 1 A ==&gt; B



RX(1) RCT A 25116-00-1  
 RGT C 1310-58-3 KOH, D 7722-84-1 H2O2  
 PRO B 1769-24-0  
 SOL 7732-18-5 Water  
 NTE Classification: Condensation; Heterocycle formation;  
 Cyclisation; Hydration; # Conditions: KOH H2O2 H2O; 30-45 deg  
 15mn

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SINCE FILE	TOTAL
ENTRY	SESSION
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